C13.22/...
Main

Volume 72B
Number 1
Jan.–Mar. 1968

MIAMI UNIVERSITY LIBRARY

Mathematical Sciences

JUL 1 1968

Formerly—
Mathematics and
Mathematical Physics

U.S. DEPARTMENT
OF COMMERCE

SECTION B

JOURNAL OF RESEARCH

NATIONAL BUREAU OF STANDARDS

Journal of Research

of the

National Bureau of Standards

B. Mathematical Sciences
(Formerly Mathematical and Mathematical Physics)

JAN.–MAR. • 1968

VOLUME • 72B

NUMBER • 1

Editor: Morris Newman

Associate Editors: John J. Sopka, F. W. Olver, and J. R. Edmonds

Publication dates: Mar. 10, June 10, Sept. 10, Dec. 10, 1968

JOURNAL OF RESEARCH

The National Bureau of Standards Journal of Research reports research and development in the fields of activity shown at right. Also included from time to time are survey articles on topics closely related to the Bureau's scientific and technical program.

The Journal is published in three separate sections as follows:

A. Physics and Chemistry

Contains papers of interest primarily to scientists working in these fields. Issued six times a year. Annual subscription: domestic, $5.00; foreign, $6.00. Single copy $1.00.

B. Mathematical Sciences

Presents studies and compilations designed mainly for the mathematician and the theoretical physicist. Issued quarterly. Annual subscription: domestic, $2.25; foreign, $2.75. Single copy 75c.

C. Engineering and Instrumentation

Reports research and development results of interest chiefly to the engineer and the applied scientist. Issued quarterly. Annual subscription: domestic, $2.75; foreign, $3.50. Single copy 75c.

The National Bureau of Standards is a principal focal point in the Federal Government for assuring maximum application of the physical and engineering sciences to the advancement of technology in industry and commerce. Its responsibilities include development and maintenance of the national standards of measurement, and the provisions of means for making measurements consistent with those standards; determination of physical constants and properties of materials; development of methods for testing materials, mechanisms, and structures, and making such tests as may be necessary, particularly for government agencies; cooperation in the establishment of standard practices for incorporation in codes and specifications; advisory service to government agencies on scientific and technical problems; invention and development of devices to serve special needs of the Government; assistance to industry, business and consumers in the development and acceptance of commercial standards and simplified trade practice recommendations; administration of programs in cooperation with United States business groups and standards organizations for the development of international standards of practice; and maintenance of a clearinghouse for the collection and dissemination of scientific, technical, and engineering information. The scope of the Bureau's activities is suggested in the following listing of its three Institutes and their organizational units.

Institute for Basic Standards. Applied Mathematics. Electricity. Metrology. Mechanics. Heat. Atomic Physics. Physical Chemistry. Radiation Physics. Laboratory Astrophysics.* Radio Standards Laboratory:* Radio Standards Physics; Radio Standards Engineering. Office of Standard Reference Data.

Institute for Materials Research. Analytical Chemistry. Metallurgy. Reactor Radiations. Polymers. Inorganic Materials. Cryogenics.* Office of Standard Reference Materials.

Institute for Applied Technology. Building Research. Electronic Instrumentation. Technical Analysis. Center for Computer Sciences and Technology. Textile and Apparel Technology Center. Office of Weights and Measures. Office of Engineering Standards Services. Office of Invention and Innovation. Office of Vehicle Systems Research. Clearinghouse for Federal Scientific and Technical Information.** Materials Evaluation Laboratory. NBS/GSA Testing Laboratory.

*Located at Boulder, Colorado 80302.
**Located at 5185 Port Royal Road, Springfield, Virginia 22151.

U.S. DEPARTMENT OF COMMERCE
C. R. Smith, Secretary
NATIONAL BUREAU OF STANDARDS
A. V. Astin, Director

Order all publications from the Superintendent of Documents
U.S. Government Printing Office, Washington, D.C. 20402

Use of funds for printing this publication approved by the Director of the Bureau of the Budget (June 22, 1966).

Preface

With this issue the name of Section B of the Journal of Research of the National Bureau of Standards is changed from "Mathematics and Mathematical Physics" to "Mathematical Sciences." The new name reflects more accurately the interests of the Bureau and the scope and breadth of the articles appearing in this Section, and includes pure mathematics, mathematical physics, numerical analysis, computation and the preparation of programs for digital computers, operations research and game theory, statistics, logic, etc.

From time to time, the Editor will solicit mathematical articles on significant advances in these disciplines from recognized authorities outside the National Bureau of Standards. He will also occasionally solicit expository articles that explain to the nonspecialist various important and difficult areas of mathematics that are relevant to the Bureau's mission. Articles solicited from outside the Bureau will be refereed by experts (both Bureau and outside) in the customary way.

A uniform single column format has been adopted, since this is more suitable to the requirements of mathematical typesetting and formula display than the old double column format.

Section B will continue as a quarterly, although two consecutive issues may be combined and issued singly from time to time.

Morris Newman

JOURNAL OF RESEARCH of the National Bureau of Standards—B. Mathematical Sciences
Vol. 72B, No. 1, January–March 1968

Means and the Minimization of Errors*

Michael Aissen**

(January 3, 1968)

Let $0 < a < b$. How should a number p be chosen so that the maximum 'relative error' obtained, by replacing a number x varying in the closed interval $[a, b]$, by p, is a minimum? For a large number of 'relative errors,' p must be chosen as the geometric mean of a and b.

Key Words: Arithmetic mean, geometric mean, harmonic mean, means, relative error.

Let $0 < a < b$. If x is a number contained in the closed interval $[a, b]$, there are various measures of the "error" committed in replacing x by an approximation p. For example the "absolute error" $|p-x|$, or the "relative error" $\frac{|p-x|}{x}$. In [1],[1] Huntington suggests more general relative errors of the form $\frac{|p-x|}{\phi(p, x)}$ where $\phi(p, x)$ is a mean of p and x (that is for all p and x, $\phi(p, x)$ lies between (not necessarily strictly) p and x). We shall consider errors of this type subject to a few other conditions. If $E(p, x) = \frac{|p-x|}{\phi(p, x)}$ is given, for each p in $[a, b]$, let $\lambda(p) = \max_x E(p, x)$ and let μ in $[a, b]$ satisfy $\lambda(\mu) = \min_p \lambda(p)$. The conditions we impose on ϕ besides being a mean are that $\lambda(p)$ exist and that μ exist and be unique. If ϕ^* denotes the 'transpose' of $\phi(\phi^*(p, x) = \phi(x, p))$, we will also require that ϕ^* satisfy the same conditions as ϕ. In [2], Pólya showed that for $\phi(p, x) = x$, $\mu = \frac{2ab}{a+b}$. In this note we compute μ for a variety of other means. As a final condition imposed on ϕ and hence on E, we demand that if p' is strictly between p and x then $E(p', x)$ be strictly smaller than $E(p, x)$ and that $E(x, x) = 0$. A set of sufficient conditions on ϕ to ensure all these requirements are

(1) ϕ is a mean.
(2) ϕ is continuous on the boundary of the square, $[a, b] \times [a, b]$.
(3) $\phi(t, u)$ and $\phi(u, t)$ as functions of u are monotone in each of the intervals $[a, t]$ and $[t, b]$, for each $t \in [a, b]$. (A)

Under the conditions assumed in paragraph 1 preceding (A),

$$\lambda(p) = \max\,(E(p, a), E(p, b)). \tag{1}$$

and μ can be characterized as the unique zero in $[a, b]$ of the equation

$$E(\mu, a) = E(\mu, b) \tag{2}$$

or

$$(\mu - a)\phi(\mu, b) + (\mu - b)\phi(\mu, a) = 0 \tag{3}$$

*An invited paper.
**Fordham University and Aerospace Research Laboratories, U.S. Air Force, Wright-Patterson Air Force Base, Ohio 45433.
[1] Figures in brackets indicate the literature references at the end of this paper.

For many choices of ϕ the solution of (3) is completely routine and we merely record the results for some of them. By $A(u, v)$, $G(u, v)$, and $H(u, v)$ we mean the arithmetic mean, geometric mean, and harmonic mean of u and v, respectively.

TABLE 1.

$\phi(p, x)$	$\mu(a, b)$
x	$H(a, b)$
p	$A(a, b)$
$\max(p, x)$	$G(a, b)$
$\min(p, x)$	$G(a, b)$
$A(p, x)$	$G(a, b)$
$G(p, x)$	$G(a, b)$
$H(p, x)$	$G(a, b)$

We discuss another example in some detail. Let

$$\phi_\tau(p, x) = A(p, x) + \frac{\tau}{2}(p - x). \tag{4}$$

For $-1 \leqq \tau \leqq 1$, ϕ_τ is admissible for our discussion. If $\mu_\tau(a, b)$ is the corresponding value of μ, (3) becomes

$$Q_\tau(\mu_\tau) = 0 \tag{5}$$

where

$$Q_\tau(u) = (\tau+1)u^2 - \tau(a+b)u + (\tau-1)ab, \tag{6}$$

or equivalently

$$Q_\tau(u) = \tau(u-a)(u-b) + u^2 - ab. \tag{7}$$

From (7), $Q_\tau(a) = a(a-b) < 0$ and $Q_\tau(b) = b(b-a) > 0$. Since Q_τ is of degree at most 2, there is a unique zero in the interval $[a, b]$. For $-1 \leqq \tau \leqq 1$, this would follow from the general theory, but the argument just presented does not depend on ϕ_τ being a mean. For all real τ we define $\mu_\tau(a, b)$ as the unique zero of (5) in the interval $[a, b]$.

From (7) it follows that

$$Q_{\tau+\delta}(u) - Q_\tau(u) = \delta(u-a)(u-b).$$

Setting $u = \mu_\tau$, for $\delta > 0$, we obtain $Q_{\tau+\delta}(\mu_\tau) < 0$. Since $Q_{\tau+\delta}(b) > 0$, we obtain $a < \mu_\tau < \mu_{\tau+\delta} < b$. Hence as a function of τ, μ_τ is strictly increasing. As $\tau \to +\infty$, one of the zeros of (5) approaches b and the other becomes unbounded. By the monotonicity we then have $\mu_\tau(a, b) \to b$ as $\tau \to +\infty$. Similarly $\mu_\tau(a, b) \to a$ as $\tau \to -\infty$. This motivates the definitions $\mu_\infty(a, b) = +b$, $\mu_{-\infty}(a, b) = a$.

We may uniquely extend μ_τ for all pairs of positive numbers by defining $\mu_\tau(x, x) = x$ and insisting that $\mu_\tau(x, y) = \mu_\tau(y, x)$. With these extensions μ is continuous in all variables $-\infty \leqq \tau \leqq \infty$, $0 < x < \infty$, $0 < y < \infty$.

It is interesting to compare this one parameter family of means with the standard means $M_\tau(a, b)$ [3]. For $\tau = -\infty, -1, 0, 1, \infty$; $\mu_\tau = M_\tau$, each is homogeneous and symmetric. For $\tau = 2$, $\mu_2(a, b) \leqq M_2(a, b)$ for all (a, b). We conjecture that for each τ, μ_τ and M_τ are comparable.

From (6) or (7) we find that if $x \neq 0$

$$x^2 Q_{-\tau}\left(\frac{ab}{x}\right) = -abQ_\tau(x). \tag{8}$$

Also

$$a \leqslant x \leqslant b \rightarrow a \leqslant \frac{ab}{x} \leqslant b. \tag{9}$$

Hence

$$\mu_{-\tau}(a, b) = \frac{ab}{\mu_\tau(a, b)}. \tag{10}$$

For $\tau = 1$, this is the elementary property

$$G(A(a, b), H(a, b)) = G(a, b). \tag{11}$$

From (4) it follows that $\phi_{-\tau} = \phi_\tau^*$. This suggests the following generalization of (10). We recall that a mean ϕ is homogeneous if for positive x, y, and k,

$$\phi(kx, ky) = k\phi(x, y).$$

THEOREM: *Let ϕ be a homogeneous mean satisfying the conditions (A). Let ϕ^* be the transposed mean. If μ and μ^* are the corresponding means of* a *and* b, *then*

$$\mu\mu^* = \text{ab}.$$

PROOF: μ is characterized by

(i) $a < \mu < b$

(ii) $(\mu - a)\phi(\mu, b) + (\mu - b)\phi(\mu, a) = 0.$

μ^* is characterized by

(iii) $a < \mu^* < b$

(iv) $(\mu^* - a)\phi^*(\mu^*, b) + (\mu^* - b)\phi^*(\mu^*, a) = 0.$

Let

$$P(x) = (x - a)\phi^*(x, b) + (x - b)\phi^*(x, a)$$

$$P\left(\frac{ab}{\mu}\right) = \left(\frac{ab}{\mu} - a\right)\phi^*\left(\frac{ab}{\mu}, b\right) + \left(\frac{ab}{\mu} - b\right)\phi^*\left(\frac{ab}{\mu}, a\right).$$

Since ϕ is homogeneous, $\phi^*\left(\frac{ab}{\mu}, b\right) = \phi\left(b, \frac{ab}{\mu}\right) = \frac{b}{\mu}\phi(\mu, a)$ and $\phi^*\left(\frac{ab}{\mu}, a\right) = \frac{a}{\mu}\phi(\mu, b)$.

Hence

$$P\left(\frac{ab}{\mu}\right) = \frac{b}{\mu}\left(\frac{ab}{\mu} - a\right)\phi(\mu, a) + \frac{a}{\mu}\left(\frac{ab}{\mu} - b\right)\phi(\mu, b)$$

$$= -\frac{1}{\mu^2}ab\{(\mu - b)\phi(\mu, a) + (\mu - a)\phi(\mu, b)\} = 0.$$

Since $a < \mu < b$, $a < \frac{ab}{\mu} < b$.

Hence $\mu^* = \frac{ab}{\mu}$ or $\mu\mu^* = ab$.

COROLLARY: *If in addition to the hypotheses of the theorem, ϕ is symmetric, ($\phi = \phi^*$), then* $\mu = G(a, b)$.

The corollary explains the frequent occurrence of $G(a, b)$ in table 1. Symmetry without homogeneity is not sufficient for $\mu(a, b) = G(a, b)$. For an example let $\phi(p, x) = \frac{p^2 + x^2}{p^2 + x^2 + 1} \max (p, x) + \frac{1}{p^2 + x^2 + 1} \min (p, x)$. By direct substitution in (3) it can be shown that $G(a, b)$ is not $\mu(a, b)$.

References

[1] Huntington, E. V., The apportionment of representatives in Congress, Trans. Amer. Math. Soc. **30,** 86 (1928).

[2] Polya, G., On the harmonic mean of two numbers, Amer. Math. Monthly, **57,** 26–28 (1950).

[3] Hardy, G. H., Littlewood, J., and Polya, G., Inequalities, 2nd Edition, pp. 12–15 (Cambridge University Press, London, 1952).

(Paper 72B1–252)

JOURNAL OF RESEARCH of the National Bureau of Standards – B. Mathematical Sciences
Vol. 72B, No. 1 January–March 1968

On Taylor's Theorem*

O. Shisha**

(December 12, 1967)

A simple way of looking at and proving Taylor's theorem.

Key Words: Iterated integrals, remainders, Taylor series.

Let $-\infty < a < b < \infty$, n an integer > 1, and f a real function with $f^{(n)}$ continuous on the closed interval $[a, b]$. Consider the number

$$I = \int_a^b \int_a^{t_n} \cdots \int_a^{t_3} \int_a^{t_2} f^{(n)}(t_1)\, dt_1 dt_2 \cdots dt_n. \tag{1}$$

Performing the integrations, one obtains

$$I = f(b) - \sum_{k=0}^{n-1} \frac{f^{(k)}(a)}{k!} (b-a)^k, \tag{2}$$

a Taylor formula with "remainder" I. To obtain the Lagrange form of the remainder, observe that taking $f(x) \equiv (x-a)^n/n!$, we have by (1) and (2),

$$I_0 = \int_a^b \int_a^{t_n} \cdots \int_a^{t_2} dt_1 dt_2 \cdots dt_n = \frac{(b-a)^n}{n!}.$$

Returning to our original f, let $M = \max_{a \le x \le b} f^{(n)}(x)$, $m = \min_{a \le x \le b} f^{(n)}(x)$. Then clearly $mI_0 \le I \le MI_0$, and unless $f^{(n)}$ is constant on $[a, b]$, strict inequalities hold. Therefore, there exists a c, $a < c < b$, such that $I/I_0 = f^{(n)}(c)$, and so

$$f(b) = \left[\sum_{k=0}^{n-1} \frac{f^{(k)}(a)}{k!} (b-a)^k\right] + \frac{f^{(n)}(c)}{n!} (b-a)^n.$$

REMARK: The usual proof of Taylor's theorem using integration by parts gives as the value of the right-hand side of (2) the number $\int_a^b f^{(n)}(t) \frac{(b-t)^{n-1}}{(n-1)!} dt$, which must therefore equal the right-hand side of (1). The equality is also evident from the known representation of an iterated indefinite integral as a single integral.

(Paper 72B1–253)

*An invited paper.
**Department of the Air Force Aerospace Research Laboratories (OAR), Wright-Patterson Air Force Base, Ohio 45433.

JOURNAL OF RESEARCH of the National Bureau of Standards – B. Mathematical Sciences
Vol. 72B, No. 1, January–March 1968

Principal Submatrices III: Linear Inequalities*

R. C. Thompson**

(December 12, 1967)

Let H be an $n \times n$ Hermitian matrix with eigenvalues $\lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_n$. Let $H(i|i)$ denote the principal submatrix of H obtained by deleting row i from H. Let $\xi_{i1} \leq \xi_{i2} \leq \ldots \leq \xi_{i,n-1}$ be the eigenvalues of $H(i|i)$. The famous Cauchy inequalities assert that $\xi_{i1}, \ldots, \xi_{i,n-1}$ interlace $\lambda_1, \ldots, \lambda_n$. It was recently proved by the present author that, for each fixed j, the arithmetic mean $n^{-1}\sum_{i=1}^{n} \xi_{ij}$ of the ξ_{ij} lies between $(1-\theta)\lambda_j + \theta\lambda_{j+1}$ and $\theta\lambda_j + (1-\theta)\lambda_{j+1}$, where $\theta = 1/n$. In the present paper the cases of equality in these inequalities for the arithmetic mean of the ξ_{ij} are discussed.

Key Words: Cauchy inequalities, Hermitian matrices, interlacing theorems, matrices, matrix inequalities, matrix theory, principal submatrices.

1. Introduction

This paper is the third in a series of papers in which the principal submatrices of a matrix are studied. In the first paper [1][1] in this series a large number of inequalities involving the eigenvalues of all of the principal $(n-1) \times (n-1)$ submatrices of a normal or Hermitian $n \times n$ matrix H were derived. In the second paper [2] certain of the inequalities obtained in [1] for Hermitian H were examined for cases of equality. The inequalities studied in [2] involved the eigenvalues of the principal submatrices in a quadratic fashion, hence we chose to call these inequalities *quadratic inequalities*. In [1] inequalities involving the eigenvalues of the principal $(n-1)$-square submatrices of Hermitian H in a linear fashion were obtained (see (2) below). These are the *linear inequalities* referred to in the title of this paper. It is the purpose of this paper to discuss cases of equality in these linear inequalities. Most of our results are obtained under the assumption that H has only simple eigenvalues. However, our most important result, Theorem 10, which characterizes those Hermitian H for which every one of our linear inequalities can achieve equality, does not require the assumption that H has simple eigenvalues. Theorem 10 produces a rather unusual condition which essentially requires that the eigenvalues of H be roots of a polynomial closely linked to the Legendre polynomials.

Certain of our results are valid for real symmetric matrices. Our most important tools are Theorems 1 and 2 of [2]. In general, when our proofs use Theorem 2 of [2] we obtain results valid for both the Hermitian and the real symmetric situations. When Theorem 1 of [2] is required, we obtain results valid only in the Hermitian situation.

2. Notation

We assume throughout this paper that $H = UDU^{-1}$ where U is unitary and $D = \text{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n)$. Except in section 5, we suppose $\lambda_1 < \lambda_2 < \ldots < \lambda_n$. In section 5, we only require that $\lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_n$. Let $H(i|i)$ be the principal submatrix of H obtained by deleting row i and

*An invited paper. The preparation of this paper was supported in part by the U.S. Air Force, Office of Scientific Research, under Grant 698-67.
**Department of Mathematics, University of California, Santa Barbara, California 93106.
[1] Figures in brackets indicate the literature reference at the end of this paper.

column i of H. Let $\xi_{i1} \leq \xi_{i2} \leq \ldots \leq \xi_{i,n-1}$ be the eigenvalues of $H(i|i)$. The famous Cauchy inequalities assert that

$$\lambda_1 \leq \xi_{i1} \leq \lambda_2 \leq \xi_{i2} \leq \ldots \leq \lambda_{n-1} \leq \xi_{i,n-1} \leq \lambda_n.$$

We say ξ_{ij} belongs to the interval $[\lambda_j, \lambda_{j+1}]$. Let

$$_jA_{j+1} = n^{-1} \sum_{i=1}^{n} \xi_{ij}.$$

In [1] the following inequalities were derived:

$$(n-1)n^{-1}\lambda_j + n^{-1}\lambda_{j+1} \leq {}_jA_{j+1} \leq n^{-1}\lambda_j + (n-1)n^{-1}\lambda_{j+1}, \qquad 1 \leq j < n. \tag{2}$$

The quantities $_jA_{j+1}$ are functions of the unitary matrix U and it is the purpose of this paper to determine which of the inequalities (2) can become equality as U varies over all unitary matrices. (Thus H and U are to be variable matrices and only D is constant.) Let $U = (u_{ij})_{1 \leq i,\, j \leq n}$. The following fundamental formula was derived both in [1] and [2].

$$f_{(i)}(\lambda) = \sum_{t=1}^{n} |u_{it}|^2 f(\lambda)/(\lambda - \lambda_t). \tag{3}$$

Here

$$f(\lambda) = \prod_{i=1}^{n} (\lambda - \lambda_i) \tag{4}$$

is the characteristic polynomial of H and

$$f_{(i)}(\lambda) = \prod_{i=1}^{n-1} (\lambda - \xi_{ij}) \tag{5}$$

is the characteristic polynomial of $H(i|i)$.

We will always let P and Q be permutation matrices. The symbol $+$ denotes direct sum.

3. Individual Cases of Equality

THEOREM 1. *Let* j *be fixed,* $1 \leq j < n$. *Then unitary* U *exists such that*

$$_jA_{j+1} = (n-1)n^{-1}\lambda_j + n^{-1}\lambda_{j+1}, \tag{6}$$

if and only if

$$f''(\lambda_j) f'(\lambda_j) \leq 0. \tag{7}$$

PROOF. We first of all remind the reader of the derivation of (2). From (3) we obtain on setting $\lambda = \lambda_j$ that

$$|u_{ij}|^2 = \left\{ \prod_{t=1}^{j-2} \frac{\lambda_j - \xi_{it}}{\lambda_j - \lambda_t} \right\} \left\{ \frac{\lambda_j - \xi_{i,j-1}}{\lambda_j - \lambda_{j-1}} \right\} \left\{ \frac{\xi_{ij} - \lambda_j}{\lambda_{j+1} - \lambda_j} \right\} \left\{ \prod_{t=j+1}^{n} \frac{\xi_{it} - \lambda_j}{\lambda_{t+1} - \lambda_j} \right\}. \tag{8}$$

(Certain of the factors in (8) are absent if $j=1, 2, n-1$, or n.) Because of the Cauchy inequalities, each fraction in (8) lies between zero and one, hence deleting all but one of the fractions in (8) increases the value of the expression. Thus from $\sum_{i=1}^{n} |u_{ij}|^2 = 1$ we obtain

$$\sum_{i=1}^{n} \frac{\lambda_j - \xi_{i,j-1}}{\lambda_j - \lambda_{j-1}} \geqslant 1, \tag{9}$$

$$\sum_{i=1}^{n} \frac{\xi_{ij} - \lambda_j}{\lambda_{j+1} - \lambda_j} \geqslant 1. \tag{10}$$

These inequalities (10), (9) are equivalent, respectively, to the first and second of the inequalities (2) after rearrangement of the terms.

Now (6) will be true if and only if the inequality (10) is equality. If $\xi_{ij} - \lambda_j \neq 0$, then equality in (10) can hold only if each of the fractions deleted from (8) is one. Hence

$$\xi_{i1} = \lambda_1, \ldots, \xi_{i,j-1} = \lambda_{j-1}, \xi_{i,j+1} = \lambda_{j+2}, \ldots, \xi_{i,n-1} = \lambda_n.$$

Using (8), it is easy to see that $u_{i1} = \ldots = u_{i,j-1} = u_{i,j+2} = \ldots = u_{in} = 0$. Thus row i of U is zero outside columns j and $j+1$. If $\xi_{ij} - \lambda_j \neq 0$ for three values of i, say $i = i_1, i_2, i_3$, then rows i_1, i_2, i_3 of U would behave as 2-tuples, hence would be dependent. This is a contradiction because U is non-singular. Thus $\xi_{ij} - \lambda_j \neq 0$ for at most two values of i, and when $\xi_{ij} - \lambda_j \neq 0$, row i of U is zero except for u_{ij} and (perhaps) $u_{i,j+1}$.

CASE (i): $\xi_{ij} - \lambda_j \neq 0$ for exactly one value of i, say $i = i_1$. In this case we must have $|u_{i_1 j}| = 1$, hence $u_{i_1, j+1} = 0$. Thus U is essentially composed of a 1-square block and an $(n-1)$ square block. After passing from $H = UDU^{-1}$ to $PHP^{-1} = (PUQ)(Q^{-1}DQ)(PUQ)^{-1}$, as in [2], we may assume

$$H = \lambda_j \dot{+} H_2 \tag{11}$$

where H_2 is $(n-1)$-square and has $\lambda_1, \ldots, \lambda_{j-1}, \lambda_{j+1}, \ldots, \lambda_n$ as eigenvalues. Moreover, we now have $\xi_{1j} - \lambda_j \neq 0$ and $\xi_{ij} - \lambda_j = 0$ for all $i > 1$. For $i > 1$ it follows from the form (11) of H that the eigenvalues of $H(i|i)$ are

$$\delta_{i1}, \delta_{i2}, \ldots, \delta_{i,j-2}; \delta_i, \lambda_j; \delta_{i,j+1}, \ldots, \delta_{i,n-1}, \tag{12}$$

where

$$\delta_{i1}, \delta_{i2}, \ldots, \delta_{i,j-2}, \delta_i, \delta_{i,j+1}, \ldots, \delta_{i,n-1} \tag{13}$$

interlace $\lambda_1, \lambda_2, \ldots, \lambda_{j-1}, \lambda_{j+1}, \ldots, \lambda_n$. Here in (12), the terms $\delta_{i1}, \ldots, \delta_{i,j-2}, \delta_i$ are absent when $j=1$. When $j=2$ the terms $\delta_{i1}, \ldots, \delta_{i,j-2}$ are absent but δ_i is present. When $j = n-1$, δ_i is present but $\delta_{i,j+1}, \ldots, \delta_{i,n-1}$ are absent.

We now show that with H in the form (11), the equation (6) for $j=1$ is valid. For with $j=1$ we have $\xi_{11} = \lambda_2$ and $\xi_{i1} = \lambda_1$ for $i > 1$, and hence (6) holds for $j=1$.

For $j \neq 1$ we require $\xi_{ij} = \lambda_j$ for all $i > 1$. From (12) it is clear that this can happen only if $\delta_i \leqslant \lambda_j$. Moreover if $\delta_i \leqslant \lambda_j$ and H is in the form (11), the equation (6) is valid, since then $\xi_{ij} = \lambda_j$ for all $i \geqslant 2$, and $\xi_{1j} = \lambda_{j+1}$ (because $H(1|1)$ has eigenvalues $\lambda_1, \ldots, \lambda_{j-1}, \lambda_{j+1}, \ldots, \lambda_n$).

Thus in Case (i) for (6) to hold it is necessary and sufficient that $\delta_i \leqslant \lambda_j$ for all $i \geqslant 2$ when $j \neq 1$. By an application of [2, Theorem 2] to H_2 and the interval $[\lambda_{j-1}, \lambda_{j+1}]$, we find that a unitary similarity of H_2 exists such that (6) holds if and only if

$$\begin{cases} \lambda_j \geqslant \text{the root of } \dfrac{d}{d\lambda} \displaystyle\prod_{\substack{t=1 \\ t \neq j}}^{n} (\lambda - \lambda_t) \text{ in interval } (\lambda_{j-1}, \lambda_{j+1}), & j \neq 1; \\ \\ \text{no condition if } j = 1. \end{cases} \tag{14}$$

Now, by a graphical argument using the fact that $\lambda_j \epsilon (\lambda_{j-1}, \lambda_{j+1})$, (14) holds if and only if

$$\begin{cases} \operatorname{sgn} \dfrac{d}{d\lambda} \prod_{\substack{t=1 \\ t \neq j}}^{n} (\lambda - \lambda_t)|_{\lambda=\lambda_j} = -\operatorname{sgn} \prod_{\substack{t=1 \\ t \neq j}}^{n} (\lambda - \lambda_t)|_{\lambda=\lambda_j} \text{ or } 0, & j \neq 1; \\ \text{no condition if } j=1. \end{cases} \tag{15}$$

It is not difficult to see that (15) for $j \neq 1$ is equivalent to $\operatorname{sgn} f''(\lambda_j) = -\operatorname{sgn} f'(\lambda_j)$ or 0, which in turn is equivalent to (7) for $j \neq 1$. For $j=1$, (15) imposes no condition and (7) is true. This completes Case (i).

CASE (ii): Here $\xi_{ij} - \lambda_j \neq 0$ for exactly two values of i, say $i=i_1$ and $i=i_2$. Thus rows i_1, i_2 of U are zero outside columns j and $j+1$, hence U essentially splits into a 2×2 block and an $(n-2) \times (n-2)$ block. If we pass from H to $PHP^{-1} = (PUQ)(Q^{-1}DQ)(PUQ)^{-1}$ as before, we may (after a change of notation) take H in the form

$$H = H_1 \dotplus H_2, \tag{16}$$

where

$$H_1 = \begin{bmatrix} a & b \\ \bar{b} & c \end{bmatrix} \tag{17}$$

has eigenvalues λ_j, λ_{j+1}, and H_2 has eigenvalues $\lambda_1, \ldots, \lambda_{j-1}, \lambda_{j+2}, \ldots, \lambda_n$. Moreover, we must now have $\xi_{ij} = \lambda_j$ for all $i > 2$. Since H_1 has eigenvalues λ_j, λ_{j+1} we have $\lambda_j \leq a$, $c \leq \lambda_{j+1}$ and

$$a + c = \lambda_j + \lambda_{j+1}.$$

With H in the form (16), the eigenvalues of $H(i|i)$ for $i > 2$ are

$$\delta_{i1}, \ldots, \delta_{i,j-2}; \delta_i, \lambda_j, \lambda_{j+1}; \delta_{i,j+2}, \ldots, \delta_{i,n-1}, \tag{18}$$

where $\delta_{i1}, \ldots, \delta_{i,j-2}, \delta_i, \delta_{i,j+2}, \ldots, \delta_{i,n-1}$ interlace $\lambda_1, \ldots, \lambda_{j-1}, \lambda_{j+2}, \ldots, \lambda_{n-1}$. For $j=1$, the terms $\delta_{i1}, \ldots, \delta_{i,j-2}, \delta_i$ are absent in (18). For $j=2$, $\delta_{i1}, \ldots, \delta_{i,j-2}$ are absent but δ_i is present. For $j=n-1$, $\delta_i, \delta_{i,j+2}, \ldots, \delta_{i,n-1}$ are all absent. For $j=n-2$, δ_i is present but $\delta_{i,j+2}, \ldots, \delta_{i,n-1}$ are all absent.

We now show that with H in the form (16), the equation (6) for $j=1$ is valid. This is so because for $j=1$ we have $\xi_{11}=c$, $\xi_{21}=a$, $\xi_{i1}=\lambda_1$ for $i>1$, and $c+a=\lambda_1+\lambda_2$.

We note also that if $n=2$ we are dealing with the case $j=1$ (since $j \leq n-1$). So let $n>2$.

We next show that for $j \neq 1$ in Case (*ii*) we must have $j \neq n-1$. For if $j=n-1$ we have from (18) that $\xi_{ij} = \xi_{i,n-1} = \lambda_{j+1}$, contradicting the requirement that $\xi_{ij} = \lambda_j$. So we may suppose $j \neq n-1$. For $j \neq 1$, $j \neq n-1$, it follows from (18) that $\xi_{ij} = \lambda_j$, $(i>2)$, can hold if and only if $\delta_i \leq \lambda_j$. Moreover, if we have H in the form (16) and $\delta_i \leq \lambda_j$ for all $i>2$, then (6) is valid (since $\xi_{1j}=c$, $\xi_{2j}=a$, $\xi_{ij}=\lambda_j$ for $i>2$ and $a+c=\lambda_j+\lambda_{j+1}$). By an application of [2, Theorem 1] to H_2 for the interval $[\lambda_{j-1}, \lambda_{j+2}]$, we find that a unitary similarity of H_2 exists such that (6) holds if and only if

$$\begin{cases} \lambda_j \geq \text{the root of } \dfrac{d}{d\lambda} \prod_{t \neq j, j+1}^{n} (\lambda - \lambda_t) \text{ in the interval } (\lambda_{j-1}, \lambda_{j+2}), \\ \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad j \neq 1, n-1; \\ \text{no condition if } j=1. \end{cases} \tag{19}$$

The condition (19) is therefore necessary and sufficient for equality (6) to hold in Case (ii).

We now show that the condition (19) of Case (ii) implies the condition (14) of Case (i). This is clear for $j=1$. For $j \neq 1, n-1$, we show

$$\begin{cases} \text{the root of } \dfrac{d}{d\lambda} \displaystyle\prod_{t\neq j, j+1}^{[=]}{}^{n} (\lambda - \lambda_t) \text{ in interval } (\lambda_{j-1}, \lambda_{j+2}) \\ > \text{the root of } \dfrac{d}{d\lambda} \displaystyle\prod_{t\neq j}^{[=]}{}^{n} (\lambda - \lambda_t) \text{ in interval } (\lambda_{j-1}, \lambda_{j+1}). \end{cases} \tag{20}$$

To see (20) let

$$g(\lambda)=\prod_{t\neq j}^{[=]}{}^{n} (\lambda-\lambda_t), \qquad h(\lambda)=\prod_{t\neq j, j+1}^{[=]}{}^{n} (\lambda-\lambda_t).$$

Then $g(\lambda)=(\lambda-\lambda_{j+1})h(\gamma)$. Let γ be the root of $h'(\lambda)$ in the interval $(\lambda_{j-1}, \lambda_{j+2})$. Then $g'(\gamma)=h(\gamma)$, hence $\operatorname{sgn} g'(\gamma)=\operatorname{sgn} h(\gamma)=-\operatorname{sgn} g(\lambda_j)$, which (by a graphical argument) forces γ to lie strictly between the two roots of $g'(\lambda)$ in the interval $(\lambda_{j-1}, \lambda_{j+2})$. Thus (20) is proved.

Thus in Case (ii) a condition that implies (7) holds. Hence (7) is the necessary and sufficient condition.

COROLLARY 1.

(i) *Let* (7) *be satisfied. Then* (6) *holds when* $H=P(\lambda_j \dot{+} H_2)P^{-1}$ *where* H_2 *has eigenvalues* $\lambda_1, \ldots, \lambda_{j-1}, \lambda_{j+1}, \ldots, \lambda_n$, *and (for* $j \neq 1$*) each principal* $(n-2)$*-square submatrix of* H_2 *has its eigenvalue belonging to the interval* $[\lambda_{j-1}, \lambda_{j+1}]$ *within the smaller interval* $[\lambda_{j-1}, \lambda_j]$.

(ii) *For* $j \neq n-1$, *if* λ_j *satisfies the condition* (19), *stronger than* (7) *when* $j \neq 1$, *then* (6) *holds when* $H=P(H_1 \dot{+} H_2)P^{-1}$ *where* H_1 *has eigenvalues* λ_j, λ_{j+1} *and* H_2 *has eigenvalues* $\lambda_1, \ldots, \lambda_{j-1}, \lambda_{j+2}, \ldots, \lambda_n$ *and (for* $j \neq 1$*) each principal* $(n-3)$*-square submatrix of* H_2 *has its eigenvalue belonging to interval* $[\lambda_{j-1}, \lambda_{j+2}]$ *within the smaller interval* $[\lambda_{j-1}, \lambda_j]$.

(iii) *In no ways other than those described in* (i) *and* (ii) *can* (6) *hold.*

An entirely similar argument will establish Theorem 2 and Corollary 2.

THEOREM 2. *Let* j *be fixed* $1 < j \leq n$. *Then unitary* U *exists such that*

$$_{j-1}A_j=(n-1)n^{-1}\lambda_j+n^{-1}\lambda_{j-1} \tag{21}$$

if and only if

$$f'(\lambda_j)f'(\lambda_j) \geq 0. \tag{22}$$

COROLLARY 2.

(i) *Let* (22) *be satisfied. Then* (21) *holds when* $H=P(\lambda_j \dot{+} H_2)P^{-1}$, *where* H_2 *has eigenvalues* $\lambda_1, \ldots, \lambda_{j-1}, \lambda_{j+1}, \ldots, \lambda_n$ *and (for* $j \neq n$*) each principal* $(n-2)$*-square submatrix of* H_2 *has its eigenvalue belonging to the interval* $[\lambda_{j-1}, \lambda_{j+1}]$ *within the smaller interval* $[\lambda_j, \lambda_{j+1}]$.

(ii) *For* $j \neq 2$, *if* λ_j *satisfies the condition*

$$\begin{cases} \lambda_j \leq \textit{the root of } \dfrac{d}{d\lambda} \displaystyle\prod_{t\neq j-1, j}^{[=]}{}^{n} (\lambda - \lambda_t) \textit{ in interval } (\lambda_{j-2}, \lambda_{j+1}), \quad j \neq n \\ \textit{no condition if } j=n. \end{cases} \tag{23}$$

(*condition* (23) *is stronger than* (22) *when* $j \neq n$), *then* (21) *holds when* $H=P(H_1 \dot{+} H_2)P^{-1}$ *where* H_1 *has eigenvalues* λ_{j-1}, λ_j, *and* H_2 *has eigenvalues* $\lambda_1, \ldots, \lambda_{j-2}, \lambda_{j+1}, \ldots, \lambda_n$ *and (for* $j \neq n$*) each principal* $(n-3)$*-square submatrix of* H_2 *has its eigenvalue belonging to the interval* $[\lambda_{j-2}, \lambda_{j+1}]$ *within the smaller interval* $[\lambda_j, \lambda_{j+1}]$.

(iii) *Other than as described in* (i), (ii), *the equality* (21) *does not hold.*

4. Simultaneous Equalities

THEOREM 3. *Let* $1 < j < k < n$. *Then*

$$_{j-1}A_j = (n-1)n^{-1}\lambda_j + n^{-1}\lambda_{j-1}, \tag{23}$$

$$_kA_{k+1} = (n-1)n^{-1}\lambda_k + n^{-1}\lambda_{k+1}, \tag{24}$$

cannot simultaneously occur.

PROOF. Suppose $\lambda_j - \xi_{i,\,j-1} \neq 0$. Then from (23), as in the proof of Theorems 1 and 2,

$$\xi_{i1} = \lambda_1, \ldots, \xi_{i,\,j-2} = \lambda_{j-2}, \xi_{i,\,j-1} \neq \lambda_j, \xi_{ij} = \lambda_{j+1}, \ldots, \xi_{ik} = \lambda_{k+1}, \ldots .$$

Hence $\xi_{ik} - \lambda_k \neq 0$ and hence, from (24),

$$\xi_{i1} = \lambda_1, \ldots, \xi_{i,\,j-2} = \lambda_{j-2}, \xi_{i,\,j-1} = \lambda_{j-1}, \xi_{ij} = \lambda_j, \ldots, \xi_{i,\,k-1} = \lambda_{k+1}, \ldots .$$

We now have the contradiction $\xi_{ij} = \lambda_{j+1}$ and $\xi_{ij} = \lambda_j$. This proves the theorem.

THEOREM 4. *Let* j *be fixed,* $1 < j < n$. *Then*

$$_{j-1}A_j = (n-1)n^{-1}\lambda_j + n^{-1}\lambda_{j-1}, \tag{25}$$

$$_jA_{j+1} = (n-1)n^{-1}\lambda_j + n^{-1}\lambda_{j+1}, \tag{26}$$

can both hold (separately or simultaneously) if and only if $f''(\lambda_j) = 0$.

PROOF. By Theorem 1, (26) can hold for some U if and only if $f''(\lambda_j)f'(\lambda_j) \leq 0$ and by Theorem 2, (25) can hold for some U if and only if $f''(\lambda_j)f'(\lambda_j) \geq 0$. Since $f'(\lambda_j) \neq 0$ as the eigenvalues of H are simple, it follows that $f''(\lambda_j) = 0$ is the necessary and sufficient for (25) and (26) to occur separately or simultaneously.

From Corollaries 1 and 2 and Theorem 4 we deduce Corollary 3.

COROLLARY 3. *Suppose* $1 < j < n$, j *fixed, and that* $f''(\lambda_j) = 0$. *Then unitary* U *exists such that both* (25) *and* (26) *hold, and in fact both* (25) *and* (26) *hold precisely when*

$$H = P(\lambda_j + H_2)P^{-1},$$

where H_2 *has engenvalues* $\lambda_1, \ldots, \lambda_{j-1}, \lambda_{j+1}, \ldots, \lambda_n$ *and each principal* $(n-2)$*-square submatrix of* H_2 *has* λ_j *as an eigenvalue.*

Theorem 4 is the $k = j$ analogue of Theorem 3. For $k = j-1$ and $n > 2$, it cannot, of course, happen that simultaneously $_{j-1}A_j$ and $_kA_{k+1}$ achieve the values $(n-1)n^{-1}\lambda_j + n^{-1}\lambda_{j-1}$ and

$$(n-1)n^{-1}\lambda_k + n^{-1}\lambda_{k+1}.$$

Here Theorem 5 answers the question of when $_{j-1}A_j = {}_kA_{k+1}$ varies over the maximal permissible set of values as U varies over all unitary matrices.

THEOREM 5. *Let* j *be fixed,* $2 \leq j \leq n$. *Then as* U *varies over all unitary matrices,* $_{j-1}A_j$ *varies over the full interval*

$$[(n-1)n^{-1}\lambda_{j-1} + n^{-1}\lambda_j,\ n^{-1}\lambda_{j-1} + (n-1)n^{-1}\lambda_j] \tag{27}$$

of permissible values allowed by the linear inequalities if and only if

$$f''(\lambda_{j-1})f'(\lambda_{j-1}) \leq 0 \text{ and } f''(\lambda_j)f'(\lambda_j) \geq 0. \tag{28}$$

PROOF. Since the roots of a polynomial are continuous functions of the coefficients of the polynomial, the function ${}_{j-1}A_j$ is a continuous function from the arcwise connected set of unitary $n \times n$ matrices to the real numbers. Thus ${}_{j-1}A_j$ covers the full interval (27) if and only if the endpoints of (27) are achievable. By Theorems 1 and 2, the endpoints of (27) are achievable if and only if the conditions (28) are satisfied.

Theorem 6 advances further the examination of ${}_{j-1}A_j$ and ${}_kA_{k+1}$ for various values of j and k that was started in Theorem 3 and continued in Theorems 4 and 5.

THEOREM 6. *Let* k, j *be fixed,* $1 \leq k, j \leq n, j \geq k+2$. *Then*

$$ {}_{j-1}A_j = (n-1)n^{-1}\lambda_j + n^{-1}\lambda_{j-1}, \tag{29} $$

$$ {}_kA_{k+1} = (n-1)n^{-1}\lambda_k + n^{-1}\lambda_{k+1}, \tag{30} $$

can simultaneously hold for some U *if and only if:*

$$ \begin{cases} \{(\lambda_k - \lambda_j)f''(\lambda_k) - 2f'(\lambda_k)\}f'(\lambda_k) \geq 0, & k \neq 1, \\ \textit{no condition if } k = 1; \end{cases} \tag{31} $$

and

$$ \begin{cases} \{(\lambda_j - \lambda_k)f''(\lambda_j) - 2f'(\lambda_j)\}f'(\lambda_j) \geq 0, & j \neq n, \\ \textit{no condition if } j = n. \end{cases} \tag{32} $$

PROOF. From (30) we find, as in the proof of Theorem 1, that $\xi_{ik} - \lambda_k \neq 0$ for exactly one or two values of i, and that when $\xi_{ik} - \lambda_k \neq 0$ then $\xi_{i1} = \lambda_1, \ldots, \xi_{i,k-1} = \lambda_{k-1}, \xi_{i,k+1} = \lambda_{k+2}, \ldots, \xi_{i,n-1} = \lambda_n$, and $u_{i1} = \ldots = u_{i,k-1} = u_{i,k+2} = \ldots = u_{in} = 0$, $u_{ik} \neq 0$. Similarly $\lambda_j - \xi_{i,j-1} \neq 0$ for at most two values of i and when $\lambda_j - \xi_{i,j-1} \neq 0$ we have $\xi_{i1} = \lambda_1, \ldots, \xi_{i,j-2} = \lambda_{j-2}, \xi_{ij} = \lambda_{j+1}, \ldots, \xi_{i,n-1} = \lambda_n$, and $u_{i1} = \ldots = u_{i,j-2} = u_{i,j+1} = \ldots = u_{in} = 0$, $u_{ij} \neq 0$. There are four cases to be considered according as $\xi_{ik} - \lambda_k$ and $\lambda_j - \xi_{i,j-1}$ are each nonzero for exactly one or two values of i. Moreover since $j - 1 \geq k + 1$, it follows from these remarks that when $\xi_{ik} - \lambda_k \neq 0$ we have $\lambda_j - \xi_{i,j-1} = 0$ and when $\lambda_j - \xi_{i,j-1} \neq 0$ we have $\xi_{ik} - \lambda_k = 0$.

CASE (i). Let $\xi_{ik} - \lambda_k \neq 0$ for exactly one value of i and let $\lambda_j - \xi_{i,j-1} \neq 0$ for exactly one value of i. We may let $\xi_{ik} = \lambda_k$ for $i \neq i_1$ and $\lambda_j = \xi_{i,j-1}$ for $i \neq i_2$. Then $i_1 \neq i_2$ and also $u_{ik} = 0$ for $i \neq i_1$, $u_{ij} = 0$ for $i \neq i_2$. Hence $|u_{i_1 k}| = 1$, $|u_{i_2 j}| = 1$, so that $u_{i_1,k+1} = 0 = u_{i_2,j-1}$. This means that U breaks down into two 1×1 blocks and an $(n-2) \times (n-2)$ block. After passing to

$$ PHP^{-1} = (PUQ)(Q^{-1}DQ)(PUQ)^{-1} $$

and changing notation, we may assume

$$ H = \lambda_k \dotplus \lambda_j \dotplus H_3 \tag{33} $$

where H_3 is $(n-2)$-square with eigenvalues

$$ \lambda_1, \ldots, \lambda_{k-1}, \lambda_{k+1}, \ldots, \lambda_{j-1}, \lambda_{j+1}, \ldots, \lambda_n. \tag{34} $$

Moreover, we now have $\xi_{ik} = \lambda_k$ for $i \neq 1$, and $\xi_{i,j-1} = \lambda_j$ for $i \neq 2$.

With H in the form (33), the eigenvalues of $H(1|1)$ are $\lambda_1, \ldots, \lambda_{k-1}, \lambda_{k+1}, \ldots, \lambda_j, \ldots, \lambda_n$, hence $\xi_{1k} = \lambda_{k+1}$ and $\xi_{1,j-1} = \lambda_j$. The eigenvalues of $H(2|2)$ are $\lambda_1, \ldots, \lambda_k, \ldots, \lambda_{j-1}, \lambda_{j+1}, \ldots, \lambda_n$, hence $\xi_{2k} = \lambda_k$ and $\xi_{2,j-1} = \lambda_{j-1}$. For $i \geq 3$, the eigenvalues of $H(i|i)$ are

$$ \delta_{i1}, \delta_{i2}, \ldots, \delta_{i,k-2}; \delta_{ik}, \lambda_k; \delta_{i,k+1}, \ldots, \delta_{i,j-2}; \delta_{ij}, \lambda_j; \delta_{i,j+1}, \ldots, \delta_{i,n-1}. \tag{35} $$

Here the numbers

$$\delta_{i1}, \ldots, \delta_{i,k-2}, \delta_{ik}, \delta_{i,k+1}, \ldots, \delta_{i,j-2}, \delta_{ij}, \delta_{i,j+1}, \ldots, \delta_{i,n-1}$$

interlace the eigenvalues (34) of H_3. In (35), the numbers $\delta_{i1}, \ldots, \delta_{i,k-2}, \delta_{ik}$ are missing when $k=1$, and when $k=2$, the numbers $\delta_{i1}, \ldots, \delta_{i,k-2}$ are missing but δ_{ik} is present. When $j=n$, the numbers $\delta_{ij}, \delta_{i,j+1}, \ldots, \delta_{i,n-1}$ are missing, and when $j=n-1$ the numbers $\delta_{i,j+1}, \ldots, \delta_{i,n-1}$ are missing but δ_{ij} is present. When $k+1=j-1$ the numbers $\delta_{i,k+1}, \ldots, \delta_{i,j-2}$ are missing but both δ_{ik} and δ_{ij} are present.

We now show that with H in the form (33), the equation (30) is valid for $k=1$. For as computed above, $\xi_{i1}=\lambda_2$, $\xi_{i1}=\lambda_1$ for all $i>1$, and this is sufficient to imply (30) when $k=1$. We also show that with H in the form (33), the equation (29) is valid for $j=n$. For as computed above, $\xi_{1,n-1}=\lambda_n$, $\xi_{2,n-1}=\lambda_{n-1}$, $\xi_{i,n-1}=\lambda_n$ for $i>2$, and this is sufficient to imply (29) when $j=n$.

For $k\neq 1$, it follows from (35) that $\xi_{ik}=\lambda_k$ for $i>2$ can hold if and only if $\delta_{ik}\leqslant\lambda_k$. For $j\neq n$ it follows from (35) that $\xi_{i,j-1}=\lambda_j$ can hold for $i>2$ if and only if $\delta_{ij}\geqslant\lambda_j$. Moreover if we have $\delta_{ik}\leqslant\lambda_k$ for all $i>2$ (when $k\neq 1$) or $\delta_{ij}\geqslant\lambda_j$ for all $i>2$ (when $j\neq n$), then using the values of ξ_{ik} or $\xi_{i,j-1}$ obtained above, we find that (30) or (29) holds, respectively. By [2, Theorem 1] we can make a unitary similarity of H_3 such that $\delta_{ik}\leqslant\lambda_k$ ($k\neq 1$) holds for all i and/or such that $\delta_{ij}\geqslant\lambda_j$ (for $j\neq n$) holds for all i, if and only if (36) and/or (37) hold:

$$\begin{cases} \lambda_k \geqslant \text{the root of } \prod_{\substack{t=1\\ t\neq k\\ t\neq j}}^{n} (\lambda-\lambda_t) \text{ in interval } (\lambda_{k-1}, \lambda_{k+1}), & k\neq 1, \\ \text{no condition if } k=1. \end{cases} \tag{36}$$

$$\begin{cases} \lambda_j \leqslant \text{the root of } \prod_{\substack{t=1\\ t\neq k\\ t\neq j}}^{n} (\lambda-\lambda_t) \text{ in interval } (\lambda_{j-1}, \lambda_{j+1}), & j\neq n, \\ \text{no condition if } j=n. \end{cases} \tag{37}$$

Thus in Case (i) the conditions (36) and (37) are the necessary and sufficient conditions for (29) and (30) both to be achievable.

We place here the first part of Corollary 4. Further parts of Corollary 4 will appear as the proof of Theorem 6 goes forward.

COROLLARY 4. (i) *Let* λ_k *and* λ_j *satisfy the conditions* (36) *and* (37). *Then both* (29) *and* (30) *hold when* $H=P(\lambda_k \dot{+} \lambda_j \dot{+} H_3)P^{-1}$, *where* H_3 *has eigenvalues* (34), *and each principal* $(n-3)$*-square submatrix of* H_3 *has its eigenvalues belonging to the intervals* $[\lambda_{k-1}, \lambda_{k+1}]$ (*for* $k\neq 1$), $[\lambda_{j-1}, \lambda_{j+1}]$ (*for* $j\neq n$) *within the smaller intervals* $[\lambda_{k-1}, \lambda_k]$, $[\lambda_j, \lambda_{j+1}]$, *respectively*.

CASE (ii). Here we assume that $\xi_{ik}-\lambda_k\neq 0$ for exactly two values of i, say $i=i_1$, and $i=i_2$, and that $\lambda_j-\xi_{i,j-1}\neq 0$ for exactly one value of i, say $i=i_3$. By remarks at the beginning of the proof, i_1, i_2, i_3 are three distinct integers. We have $|u_{i_3 j}|=1$ as $u_{ij}=0$ for $i\neq i_3$, hence $u_{i_3 t}=0$ for $t\neq j$. Thus U splits up into three nonzero blocks: a 2×2 block in rows i_1, i_2 and columns k, $k+1$; a 1×1 block at position (i_3, j); and $(n-3)\times(n-3)$ block in the rows complementary to i_1, i_2, i_3 and the columns complementary to k, $k+1$, j. After passing to $PHP^{-1}=(PUQ)(Q^{-1}DQ)(PUQ)^{-1}$, and changing notation, we may assume

$$H=H_1 \dot{+} \lambda_j \dot{+} H_3 \tag{38}$$

where H_1 has eigenvalues λ_k, λ_{k+1}, and H_3 has eigenvalues

$$\lambda_1, \ldots, \lambda_{k-1}, \lambda_{k+2}, \ldots, \lambda_{j-1}, \lambda_{j+1}, \ldots, \lambda_n. \tag{39}$$

Moreover we now have $\xi_{ik}=\lambda_k$ for $i>2$ and $\xi_{i,\,j-1}=\lambda_j$ for $i\neq 3$. Let H_1 be given by (17). Then $\lambda_k\leq a$, $c\leq\lambda_{k+1}$ and $a+c=\lambda_k+\lambda_{k+1}$.

Observe that, with H given by (38), we have $\xi_{1k}=c$, $\xi_{2k}=a$, $\xi_{1,\,j-1}=\lambda_j$, $\xi_{2,\,j-1}=\lambda_j$, $\xi_{3k}=\lambda_k$, $\xi_{3,\,j-1}=\lambda_{j-1}$. For $i>3$ the eigenvalues of $H(i|i)$ are

$$\delta_{i1},\ \ldots,\delta_{i,\,k-2};\ \delta_{ik},\lambda_k,\lambda_{k+1};\ \delta_{i,\,k+2},\ \ldots,\delta_{i,\,j-2};\ \delta_{ij},\lambda_j;\ \delta_{i,\,j+1},\ \ldots,\delta_{i,\,n-1}. \tag{40}$$

Here the numbers

$$\delta_{i1},\ \ldots,\delta_{i,\,k-2},\ \delta_{ik},\ \delta_{i,\,k+2},\ \ldots,\delta_{i,\,j-2},\ \delta_{ij},\ \delta_{i,\,j+1},\ \ldots,\delta_{i,\,n-1}$$

interlace the numbers (39). When $k=1$, the numbers $\delta_{i1},\ \ldots,\ \delta_{i,\,k-2},\ \delta_{ik}$ are absent from (40). When $k=2$, the numbers $\delta_{i1},\ \ldots,\ \delta_{i,\,k-2}$ are absent from (40) but δ_{ik} is present. When $j=n$, the numbers $\delta_{ij},\ \delta_{i,\,j+1},\ \ldots,\ \delta_{i,\,n-1}$ are absent from (40). When $j=n-1$, the numbers $\delta_{i,\,j+1},\ \ldots,\ \delta_{i,\,n-1}$ are absent from (40) but δ_{ij} is present. When $j-1>k+2$ the central set $\delta_{i,\,k+2},\ \ldots,\ \delta_{i,\,j-2}$ is present in (40). When $j-1=k+2$ the central set $\delta_{i,\,k+2},\ \ldots,\ \delta_{i,\,j-2}$ are absent but δ_{ik} and δ_{ij} are separate entities, both being present (except: δ_{ik} is absent if $k=1$ and δ_{ij} is absent if $j=n$). When $j-1=k+1$ the central set $\delta_{i,\,k+2},\ \ldots,\ \delta_{i,\,j-2}$ is absent, and δ_{ik} and δ_{ij} merge into one entity, $\delta_{ik}=\delta_{ij}$ being the eigenvalue of $H_3(i-3|i-3)$ belonging to the interval $[\lambda_{k-1},\ \lambda_{j+1}]$ (except that for $k=1$ or $j=n$, $\delta_{ik}=\delta_{ij}$ is absent).

We now show that the equation (39) for $k=1$ is valid when H has the form (38). This follows from the values ξ_{11}, ξ_{21}, ξ_{31} computed above, the fact that $a+c=\lambda_1+\lambda_2$, and the fact that (from (40)), $\xi_{i1}=\lambda_1$ for all $i>3$. We also show that the equation (29) for $j=n$ is valid when H has the form (38). This follows from the values of $\xi_{1,\,n-1}$, $\xi_{2,\,n-1}$, $\xi_{3,\,n-1}$ computed above, and the fact that (from (40)) $\xi_{i,\,n-1}=\lambda_n$ for all $i>3$.

Now note that when $n=3$ we in fact have $k=1$ and $j=3=n$. This is so since $j\geq k+2$. So assume $n>3$.

We now prove (assuming $n>3$) that $j\neq k+2$. We use (40). If $j-1=k+1$ we have: when $k=1$, $\xi_{i,\,j-1}=\xi_{i2}=\lambda_2=\lambda_{j-1}$ contrary to the requirement $\xi_{i,\,j-1}=\lambda_j$ for $i>3$; when $j=n$, $\xi_{ik}=\xi_{i,\,n-2}=\lambda_{k+1}$ contrary to the requirement $\xi_{ik}=\lambda_k$ for $i>3$; when $k\neq 1$ and $j\neq n$ in order to meet the requirement $\xi_{ik}=\lambda_k$ we must have (from (40)) that $\delta_{ik}\leq\lambda_k$, and then $\xi_{i,\,j-1}=\lambda_{k+1}\neq\lambda_j$, thus contradicting $\xi_{i,\,j-1}=\lambda_j$ for $i>3$. So we may assume $j-1>k+1$ and that δ_{ik} and δ_{ij} are distinct entities.

For $k\neq 1$ it now follows from (40) that in order for $\xi_{ik}=\lambda_k$ for $i>3$ it is necessary and sufficient that $\delta_{ik}\leq\lambda_k$. For $j\neq n$ it follows from (40) that in order for $\xi_{i,\,j-1}=\lambda_j$ for $i>3$ it is necessary and sufficient that $\delta_{ij}\geq\lambda_j$. Moreover with H in the form (38) and using values ξ_{1k}, ξ_{2k}, ξ_{3k}, $\xi_{1,\,j-1}$, $\xi_{2,\,j-1}$, $\xi_{3,\,j-1}$ obtained above, if $\xi_{ik}=\lambda_k$ for all $i>3$, $(k\neq 1)$, we find that (30) is satisfied and if $\xi_{i,\,j-1}=\lambda_j$ for all $i>3$, $(j\neq n)$, we find that (29) is satisfied. Now by [1, Theorem 1] it follows that $\delta_{ik}\leq\lambda_k$ (for $k\neq 1$) and/or $\lambda_j\leq\delta_{ij}$ (for $j\neq n$) can be achieved by some matrix unitarily similar to H_3, if and only if

$$\begin{cases}\lambda_k\geq\text{the root of }\dfrac{d}{d\lambda}\displaystyle\prod_{\substack{t=1\\ t\neq k,\,k+1,\,j}}^{n}(\lambda-\lambda_t)\text{ in interval }(\lambda_{k-1},\ \lambda_{k+2}),\ k\neq 1,\\ \text{no condition if }k=1,\end{cases} \tag{41}$$

and/or

$$\begin{cases}\lambda_j\leq\text{the root of }\dfrac{d}{d\lambda}\displaystyle\prod_{\substack{t=1\\ t\neq k,\,k+1,\,j}}^{n}(\lambda-\lambda_t)\text{ in interval }(\lambda_{j-1},\ \lambda_{j+1}),\ j\neq n,\\ \text{no condition if }j=n.\end{cases} \tag{42}$$

289-930 OL-68—2

We have thus demonstrated that in Case (ii) the conditions (41) and (42), together with $j \neq k+2$ for $n > 3$, are the necessary and sufficient conditions in order that (29) and (30) can both hold. We now complete the proof in Case (ii) by showing that for $k \neq 1$ and $j > k+2$,

$$\text{the root of } \frac{d}{d\lambda} \prod_{\substack{t=1 \\ t \neq k, k+1, j}}^{n} (\lambda - \lambda_t) \text{ in interval } (\lambda_{k-1}, \lambda_{k+2})$$

$$> \text{the root of } \frac{d}{d\lambda} \prod_{\substack{t=1 \\ t \neq k, j}}^{n} (\lambda - \lambda_t) \text{ in interval } (\lambda_{k-1}, \lambda_{k+1}) \tag{43}$$

and for $j \neq n$ and $j > k+2$,

$$\text{the root of } \frac{d}{d\lambda} \prod_{\substack{t=1 \\ t \neq k, k+1, j}}^{n} (\lambda - \lambda_t) \text{ in interval } (\lambda_{j-1}, \lambda_{j+1})$$

$$< \text{the root of } \frac{d}{d\lambda} \prod_{\substack{t=1 \\ t \neq k, j}}^{n} (\lambda - \lambda_t) \text{ in interval } (\lambda_{j-1}, \lambda_{j+1}). \tag{44}$$

If we can demonstrate (43), (44) then the conditions (41), (42) of Case (ii) imply the conditions (36) and (37) in Case (i).

Let

$$g(\lambda) = \prod_{\substack{t=1 \\ t \neq k, j}}^{n} (\lambda - \lambda_t), \qquad h(\lambda) = \prod_{\substack{t=1 \\ t \neq k, k+1, j}}^{n} (\lambda - \lambda_t).$$

Then $g(\lambda) = (\lambda - \lambda_{k+1}) h(\lambda)$. We use the fact that $k+2 \leq j-1$. Let γ be the root of $h'(\lambda)$ in the interval $(\lambda_{k-1}, \lambda_{k+2})$. Then $g'(\gamma) = h(\gamma)$ and so $\operatorname{sgn} g'(\gamma) = \operatorname{sgn} h(\gamma) = -\operatorname{sgn} g(\lambda_k)$, which forces $\gamma >$ root of $g'(\lambda)$ in interval $(\lambda_{k-1}, \lambda_{k+1})$. This proves (43). Let β be the root of $h'(\lambda)$ in the interval $(\lambda_{j-1}, \lambda_{j+1})$. Then $g'(\beta) = h(\beta)$, hence $\operatorname{sgn} g'(\beta) = \operatorname{sgn} h(\beta) = \operatorname{sgn} g(\beta)$, which forces $\beta <$ root of $g'(\lambda)$ in interval $(\lambda_{j-1}, \lambda_{j+1})$. This proves (44) and completes Case (ii).

COROLLARY 4. (ii) *Let* $j > k+2$ *except* $k = 1$, $j = 3$ *for* $n = 3$. *Then the condition* (41) *for* $k \neq 1$ *is stronger than the condition* (36) *and the condition* (42) *for* $j \neq n$ *is stronger than the condition* (37). *If both* (41) *and* (42) *are satisfied then equalities* (29) *and* (30) *are both valid when* $H = P(H_1 + \lambda_j + H_3)P^{-1}$, *when* H_1 *has eigenvalues* λ_k, λ_{k+1}, H_3 *has eigenvalues* (39), *and each principal* $(n-4)$*-square submatrix of* H_3 *has its eigenvalues belonging to the intervals* $[\lambda_{k-1}, \lambda_{k+2}]$ (*for* $k \neq 1$), $[\lambda_{j-1}, \lambda_{j+1}]$ (*for* $j \neq n$) *within the smaller intervals* $[\lambda_{k-1}, \lambda_k]$, $[\lambda_j, \lambda_{j+1}]$, *respectively*.

CASE (iii). Here we assume $\xi_{ik} - \lambda_k \neq 0$ for exactly one value of i and $\lambda_j - \xi_{i,j-1} \neq 0$ for exactly two values of i. This case is very similar to Case (ii). One gets H into the form

$$H = P(\lambda_k \dot{+} H_2 \dot{+} H_3)P^{-1} \tag{45}$$

where H_2 has eigenvalues λ_{j-1}, λ_j and H_3 has eigenvalues

$$\lambda_1, \ldots, \lambda_{k-1}, \lambda_{k+1}, \ldots, \lambda_{j-2}, \lambda_{j+1}, \ldots, \lambda_n. \tag{45'}$$

One proves that $j > k+2$ except for $k = 1$, $j = 3$ when $n = 3$. In place of (41) and (42) one obtains

$$\begin{cases} \lambda_k \geq \text{the root of } \dfrac{d}{d\lambda} \displaystyle\prod_{\substack{t=1 \\ t \neq k, j-1, j}}^{n} (\lambda - \lambda_t) \text{ in interval } (\lambda_{k-1}, \lambda_{k+1}), & k \neq 1, \\ \text{no condition if } k = 1; \end{cases} \tag{46}$$

$$\begin{cases} \lambda_j \leqslant \text{the root of } \dfrac{d}{d\lambda} \prod\limits_{\substack{t=1 \\ t\neq k,\, j-1,\, j}}^{n} (\lambda-\lambda_t) \text{ in interval } (\lambda_{j-2},\ \lambda_{j+1}), \qquad j \neq n, \\ \text{no condition if } j=n; \end{cases} \tag{47}$$

and in place of (43), (44), one obtains (48) for $k \neq 1$ and (49) for $j \neq n$:

$$\text{the root of } \frac{d}{d\lambda} \prod_{\substack{t=1 \\ t\neq k,\, j-1,\, j}}^{n} (\lambda-\lambda_t) \text{ in interval } (\lambda_{k-1},\ \lambda_{k+1})$$

$$> \text{the root of } \frac{d}{d\lambda} \prod_{\substack{t=1 \\ t\neq k,\, j}}^{n} (\lambda-\lambda_t) \text{ in interval } (\lambda_{k-1},\ \lambda_{k+1}); \tag{48}$$

$$\text{the root of } \frac{d}{d\lambda} \prod_{\substack{t=1 \\ t\neq k,\, j-1,\, j}}^{n} (\lambda-\lambda_t) \text{ in interval } (\lambda_{j-2},\ \lambda_{j+1})$$

$$< \text{the root of } \frac{d}{d\lambda} \prod_{\substack{t=1 \\ t\neq k,\, j}}^{n} (\lambda-\lambda_t) \text{ in interval } (\lambda_{j-1},\ \lambda_{j+1}). \tag{49}$$

COROLLARY 4. (iii) *Let* $j > k+2$ *except* $k=1$, $j=3$ *for* $n=3$. *Then the condition* (46) *for* $k \neq 1$ *is stronger than the condition* (36) *and the condition* (47) *for* $j \neq n$ *is stronger than the condition* (37). *If both* (46) *and* (47) *are satisfied then equalities* (29) *and* (30) *both are valid when* H *has the form* (45), *where* H_2 *has eigenvalues* λ_{j-1}, λ_j, H_3 *has eigenvalues* (45'), *and where each principal* $(n-4)$*-square submatrix of* H_3 *has its eigenvalues belonging to the intervals* $[\lambda_{k-1},\ \lambda_{k+1}]$ (*for* $k \neq 1$), $[\lambda_{j-2},\ \lambda_{j+1}]$ (*for* $j \neq n$) *within the smaller intervals* $[\lambda_{k-1},\ \lambda_k]$, $[\lambda_j,\ \lambda_{j+1}]$, *respectively*.

CASE (iv). In this case we have $\xi_{ik}-\lambda_k \neq 0$ for exactly two values of i and $\lambda_j-\xi_{i,j-1} \neq 0$ for exactly two values of i. Moreover, as before, when $\xi_{ik}-\lambda_k \neq 0$ then $\lambda_j-\xi_{i,j-1}=0$ and when $\lambda_j-\xi_{i,j-1} \neq 0$ then $\xi_{ik}-\lambda_k=0$. So we may find four integers i_1, i_2, i_3, i_4 such that $\xi_{ik}-\lambda_k=0$ for $i \neq i_1$, i_2 and $\lambda_j-\xi_{i,j-1}=0$ for $i \neq i_3$, i_4. We then have $u_{i_1 t}=0$ for $t \neq k$, $k+1$; $u_{i_2 t}=0$ for $t \neq k$, $k+1$; $u_{i_3 t}=0$ for $t \neq j-1$, j; $u_{i_4 t}=0$ for $t \neq j-1$, j. We show: $k+1 \neq j-1$. For if $k+1=j-1$, rows i_1, i_2, i_3, i_4 of U are zero except for column positions k, $k+1$, j, hence these four rows behave as 3-tuples, hence are linearly dependent. This contradiction shows that $k+1 \neq j-1$, hence $k+1<j-1$. Now rows i_1, i_2 of U are zero except for the 2×2 submatrix sitting in rows i_1, i_2 and columns k, $k+1$. Thus, as U is unitary, columns k, $k+1$ are also zero except for rows i_1, i_2. Similarly rows i_3, i_4 and columns $j-1$, j are zero except for the 2×2 submatrix sitting at the intersection of these rows and columns.

Thus we may pass to $PHP^{-1}=(PUQ)(Q^{-1}DQ)(PUQ)^{-1}$ and so, after a change of notation, assume

$$H=H_1+H_2+H_3 \tag{50}$$

where: H_1 has eigenvalues λ_k, λ_{k+1}; H_2 has eigenvalues λ_{j-1}, λ_j; H_3 has eigenvalues

$$\lambda_1, \ldots, \lambda_{k-1}, \lambda_{k+2}, \ldots, \lambda_{j-2}, \lambda_{j+1}, \ldots, \lambda_n. \tag{51}$$

We now have $\xi_{ik}=\lambda_k$ and $\xi_{i,j-1}=\lambda_j$ for $i>4$. Let H_1 be given by (17) and H_2 by

$$H_2=\begin{bmatrix} a' & b' \\ \overline{b}' & c' \end{bmatrix}.$$

Assuming H in the form (50), one easily sees that $\xi_{1k}=c$, $\xi_{1,j-1}=\lambda_j$, $\xi_{2k}=a$, $\xi_{2,j-1}=\lambda_j$, $\xi_{3k}=\lambda_k$, $\xi_{3,j-1}=c'$, $\xi_{4k}=\lambda_k$, $\xi_{4,j-1}=a'$.

For $i>4$, the eigenvalues of $H(i|i)$ are

$$\delta_{i1}, \ldots, \delta_{i,k-2}; \delta_{ik}, \lambda_k, \lambda_{k+1}; \delta_{i,k+2}, \ldots, \delta_{i,j-3}; \delta_{ij}, \lambda_{j-1}, \lambda_j; \delta_{i,j+1}, \ldots, \delta_{i,n-1}, \tag{52}$$

where

$$\delta_{i1}, \ldots, \delta_{i,k-2}, \delta_{ik}, \delta_{i,k+2}, \ldots, \delta_{i,j-3}, \delta_{ij}, \delta_{i,j+1}, \ldots, \delta_{i,n-1}$$

interlace the numbers (51). When $k=1$, the numbers $\delta_{i1}, \ldots, \delta_{i,k-2}, \delta_{ik}$ are absent in (52). When $k=2$ the numbers $\delta_{i1}, \ldots, \delta_{i,k-2}$ are absent but δ_{ik} is present. When $j=n$ the numbers δ_{ij}, $\delta_{i,j+1}, \ldots, \delta_{i,n-1}$ are absent. When $j=n-1$ the numbers $\delta_{i,j+1}, \ldots, \delta_{i,n-1}$ are absent but δ_{ij} is present. When $j=k+4$ the numbers $\delta_{i,k+2}, \ldots, \delta_{i,j-3}$ are absent but δ_{ik} and δ_{ij} are present as separate entities (except: δ_{ik} is absent if $k=1$ and δ_{ij} is absent if $j=n$). When $j=k+3$ the numbers $\delta_{i,k+2}, \ldots, \delta_{i,j-3}$ are absent and $\delta_{ik}=\delta_{ij}$ appear as a single entity (except that $\delta_{ik}=\delta_{ij}$ is absent if $k=1$ or $j=n$).

We now show that when H has the form (50), equation (30) for $k=1$ is valid. This follows from the values of $\xi_{11}, \ldots, \xi_{41}$ computed above, the fact that $a+c=\lambda_1+\lambda_2$, and the fact that $\xi_{i1}=\lambda_1$ for $i>4$ (which follows from (52) when $k=1$). We also show that equation (29) for $j=n$ is valid. This follows from the values of $\xi_{1,n-1}, \ldots, \xi_{4,n-1}$ computed above, and the fact that $a'+c'=\lambda_{n-1}+\lambda_n$, and the fact that $\xi_{i,n-1}=\lambda_n$ for $i>4$ (which follows from (52) when $j=n$).

Observe also that when $n=4$ we in fact have $k=1$ and $j=4=n$, since $j\geq k+3$. So assume $n>4$.

We now show that $j=k+3$ is impossible for $n>4$. For let $j=k+3$. We use (52). If $k=1$ then $\xi_{i,j-1}=\xi_{i,3}=\lambda_3\neq\lambda_4$ contradicting the requirement that $\xi_{i,j-1}=\lambda_j$ for $i>4$. If $j=n$ then $\xi_{ik}=\xi_{i,n-3}=\lambda_{k+1}\neq\lambda_k$ contradicting the requirement that $\xi_{ik}=\lambda_k$ for $i>4$. If $k\neq 1$, $j\neq n$, then in order that $\xi_{ik}=\lambda_k$ we must have $\delta_{ik}\leq\lambda_k$, and then $\xi_{i,j-1}=\xi_{i,k+2}=\lambda_{j-1}\neq\lambda_j$, again a contradiction for $i>4$. Thus $j\geq k+4$ as claimed, and so δ_{ik} and δ_{ij} are separate entities in (52).

For $k\neq 1$ we find from (52) that $\xi_{ik}=\lambda_k$ holds for $i>4$ if and only if $\delta_{ik}\leq\lambda_k$. For $j\neq n$ we find from (52) that $\xi_{i,j-1}=\lambda_j$ holds for $i>4$ if and only if $\delta_{ij}\geq\lambda_j$. Moreover, using values of $\xi_{1k}, \ldots, \xi_{4k}$, $\xi_{1,j-1}, \ldots, \xi_{4,j-1}$ obtained above and $a+c=\lambda_k+\lambda_{k+1}$, $a'+c'=\lambda_{j-1}+\lambda_j$, we find for $k\neq 1$ or for $j\neq n$ that if $\delta_{ik}\leq\lambda_k$ for all $i>4$ or $\delta_{ij}\geq\lambda_j$ for all $i>4$, then (30) or (29) are satisfied, respectively.

Now by an application of [2, Theorem 1] to H_3, the necessary and sufficient conditions that H_3 be unitarily similar to a matrix for which $\delta_{ik}\leq\lambda_k$ $(k\neq 1)$ and/or $\delta_{ij}\geq\lambda_j$ $(j\neq n)$ are the following conditions (53) and/or (54):

$$\begin{cases} \lambda_k \geq \text{the root of } \dfrac{d}{d\lambda}\displaystyle\prod_{\substack{t=1\\ t\neq k,\,k+1\\ t\neq j-1,\,j}}^{n}(\lambda-\lambda_t) \text{ in the interval } (\lambda_{k-1}, \lambda_{k+2}); & k\neq 1, \\ \text{no condition if } k=1, \end{cases} \tag{53}$$

$$\begin{cases} \lambda_j \leq \text{the root of } \dfrac{d}{d\lambda}\displaystyle\prod_{\substack{t=1\\ t\neq k,\,k+1\\ t\neq j-1,\,j}}^{n}(\lambda-\lambda_t) \text{ in the interval } (\lambda_{j-2}, \lambda_{j+1}); & j\neq n, \\ \text{no condition if } j=n. \end{cases} \tag{54}$$

Thus the necessary and sufficient conditions in Case (iv) that (29) and (30) can both hold are (53), (54), together with $j\geq k+4$ for $n>4$ and $k=1$, $j=4$ for $n=4$.

We now show for $j \geq k+4$:

$$\text{the root of } \frac{d}{d\lambda} \prod_{\substack{t=1 \\ t\neq k,\, k+1 \\ t\neq j-1,\, j}}^{n} (\lambda-\lambda_t) \text{ in interval } (\lambda_{k-1},\, \lambda_{k+2})$$

$$> \text{root of } \frac{d}{d\lambda} \prod_{\substack{t=1 \\ t\neq k,\, j}}^{n} (\lambda-\lambda_t) \text{ in interval } (\lambda_{k-1},\, \lambda_{k+1}); \qquad k \neq 1; \tag{55}$$

$$\text{root of } \frac{d}{d\lambda} \prod_{\substack{t=1 \\ t\neq k,\, k+1 \\ t\neq j-1,\, j}}^{n} (\lambda-\lambda_t) \text{ in interval } (\lambda_{j-2},\, \lambda_{j+1})$$

$$< \text{root of } \frac{d}{d\lambda} \prod_{\substack{t=1 \\ t\neq k,\, j}}^{n} (\lambda-\lambda_t) \text{ in interval } (\lambda_{j-1},\, \lambda_{j+1}), \qquad j \neq n. \tag{56}$$

Once (55), (56) are demonstrated it will follow that the conditions of Case (iv) imply the conditions (36), (37) of Case (i), and this will complete the demonstration that (36) and (37) are necessary and sufficient.

Let

$$g(\lambda) = \prod_{\substack{t=1 \\ t\neq k,\, j}}^{n} (\lambda-\lambda_t), \qquad h(\lambda) = \prod_{\substack{t=1 \\ t\neq k,\, k+1 \\ t\neq j-1,\, j}}^{n} (\lambda-\lambda_t).$$

Then $g(\lambda) = (\lambda-\lambda_{k+1})(\lambda-\lambda_{j-1})h(\lambda)$. Let γ be the root of $h'(\lambda)$ in the interval $(\lambda_{k-1},\, \lambda_{k+2})$. If $\gamma \geq \lambda_{k+1}$ then (55) holds. If $\gamma < \lambda_{k+1}$ then

$$\operatorname{sgn} \frac{d}{d\lambda} (\lambda-\lambda_{k+1})(\lambda-\lambda_{j-1}) \Big|_{\lambda=\gamma} = -1,$$

hence $\operatorname{sgn} g'(\gamma) = -\operatorname{sgn} h(\gamma) = -\operatorname{sgn} g(\gamma)$, which implies (55). Thus (55) holds. Let β be the root of $h'(\lambda)$ in the interval $(\lambda_{j-2},\, \lambda_{j+1})$. If $\beta \leq \lambda_{j-1}$ then (56) holds. If $\beta > \lambda_{j-1}$ then

$$\operatorname{sgn} \frac{d}{d\lambda} (\lambda-\lambda_{k+1})(\lambda-\lambda_{j-1}) \Big|_{\lambda=\beta} = +1,$$

hence $\operatorname{sgn} g'(\gamma) = \operatorname{sgn} h(\gamma) = \operatorname{sgn} g(\gamma)$, which implies (56). This completes Case (iv).

COROLLARY 4. (iv) *Let* $j \geq k+4$ *except* $k=1$, $j=4$ *for* $n=4$. *Then the condition* (53) *for* $k \neq 1$ *is stronger than the condition* (36) *and the condition* (54) *for* $j \neq n$ *is stronger than the condition* (37). *If both* (53) *and* (54) *are satisfied then equalities* (29) *and* (30) *both hold when* $H = P(H_1 \dotplus H_2 \dotplus H_3)P^{-1}$, *where* H_1 *has eigenvalues* λ_k, λ_{k+1}, H_2 *has eigenvalues* λ_{j-1}, λ_j, H_3 *has eigenvalues* (51), *and where each principal* $(n-5)$*-square submatrix of* H_3 *has its eigenvalues belonging to the intervals* $[\lambda_{k-1}, \lambda_{k+2}]$ (*for* $k \neq 1$), $[\lambda_{j-2}, \lambda_{j+1}]$ (*for* $j \neq n$) *within the smaller intervals* $[\lambda_{k-1}, \lambda_k]$, $[\lambda_j, \lambda_{j+1}]$, *respectively.*

(v) *Except as described in Corollary* 4, (i)-(iv), *the equalities* (29), (30) *do not both hold.*

To complete the proof of Theorem 6, we have to show that conditions (36) and (37) are equivalent to (31) and (32). This proof follows.

By a graphical argument one sees, for $k \neq 1$, that the condition (36) is equivalent to

$$\{f(\lambda)(\lambda-\lambda_k)^{-1}(\lambda-\lambda_j)^{-1}\}'\{f(\lambda)(\lambda-\lambda_k)^{-1}(\lambda-\lambda_j)^{-1}\} \mid_{\lambda=\lambda_k} \leq 0.$$

But

$$\{f(\lambda)(\lambda-\lambda_j)^{-1}\}'\Big|_{\lambda=\lambda_k}=\prod_{\substack{\nu=1\\ \nu\neq j\\ \nu\neq k}}^{n}(\lambda_k-\lambda_\nu)=f(\lambda)(\lambda-\lambda_k)^{-1}(\lambda-\lambda_j)^{-1}\Big|_{\lambda=\lambda_k}.$$

Also

$$\{f(\lambda)(\lambda-\lambda_j)^{-1}\}''\Big|_{\lambda=\lambda_k}=2\sum_{\substack{\mu=1\\ \mu\neq j\\ \mu\neq k}}^{n}\prod_{\substack{\nu=1\\ \nu\neq\mu\\ \nu\neq j\\ \nu\neq k}}^{n}(\lambda_k-\lambda_\nu)$$

$$=\{2f(\lambda)(\lambda-\lambda_k)^{-1}(\lambda-\lambda_j)^{-1}\}'\Big|_{\lambda=\lambda_k}.$$

But

$$\{f(\lambda)(\lambda-\lambda_j)^{-1}\}'\Big|_{\lambda=\lambda_k}=f'(\lambda_k)(\lambda_k-\lambda_j)^{-1},$$

$$\{f(\lambda)(\lambda-\lambda_j)^{-1}\}''\Big|_{\lambda=\lambda_k}=\{(\lambda_k-\lambda_j)f''(\lambda_k)-2f'(\lambda_k)(\lambda_k-\lambda_j)^{-2}.$$

Combining all these facts and using $\lambda_k-\lambda_j<0$, the equivalence of (36) and (31) follows. Similarly one establishes the equivalence of (37) and (32). This completes the proof of Theorem 6.

COROLLARY 5. *Let* $t\neq 1, n$. *If for some* $s\geq t+2$ *we have simultaneously*

$$\begin{aligned}{}_{t}A_{t+1}&=(n-1)n^{-1}\lambda_t+n^{-1}\lambda_{t+1},\\ {}_{s-1}A_{s}&=(n-1)n^{-1}\lambda_s+n^{-1}\lambda_{s-1},\end{aligned}\tag{57}$$

then for $s_1\leq t-2$ *we never have simultaneously*

$$\begin{aligned}{}_{t-1}A_{t}&=(n-1)n^{-1}\lambda_t+n^{-1}\lambda_{t-1},\\ {}_{s_1}A_{s_1+1}&=(n-1)n^{-1}\lambda_{s_1}+n^{-1}\lambda_{s_1+1},\end{aligned}\tag{58}$$

If for some $s_1\leq t-2$ *we have* (58) *simultaneously then for* $s\geq t+2$ *we never have* (57) *simultaneously. If* $f''(\lambda_t)=0$ *then for no* $s\geq t+2$ *can* (57) *both hold and for no* $s_1\leq t-2$ *can* (58) *both hold.*

PROOF. If both of eqs (57) hold then by Theorem 6 we have

$$\{(\lambda_t-\lambda_s)f''(\lambda_t)-2f'(\lambda_t)\}f'(\lambda_t)\geq 0,\tag{59}$$

and if both of eqs (58) hold then by Theorem 6 we have

$$\{(\lambda_t-\lambda_{s_1})f''(\lambda_t)-2f'(\lambda_t)\}f'(\lambda_t)\geq 0.\tag{60}$$

If $f'(\lambda_t)>0$ we obtain the contradiction

$$0<2f'(\lambda_t)(\lambda_t-\lambda_{s_1})^{-1}\leq f''(\lambda_t)\leq 2f'(\lambda_t)(\lambda_t-\lambda_s)^{-1}<0$$

and a similar contradiction is obtained if $f'(\lambda_t)<0$. If $f''(\lambda_t)=0$ it is clear that both (59) and (60) are false.

THEOREM 7. *Let* $1 < j < k \leq n$. *Then*

$$_{j-1}A_j = (n-1)n^{-1}\lambda_j + n^{-1}\lambda_{j-1}, \tag{61}$$

$$_{k-1}A_k = (n-1)n^{-1}\lambda_k + n^{-1}\lambda_{k-1} \tag{62}$$

never happen simultaneously.

PROOF. If (62) holds then from $\xi_{i,k-1} \neq \lambda_k$ we get $\xi_{i,j-1} = \lambda_{j-1}$, hence $\lambda_j - \xi_{i,j-1} \neq 0$, hence from (61) follows $\xi_{i,k-1} = \lambda_k$. We have a contradiction. This completes the proof.

Similarly one proves Theorem 8.

THEOREM 8. *Let* $1 \leq j < k < n$. *Then*

$$_jA_{j+1} = (n-1)n^{-1}\lambda_j + n^{-1}\lambda_{j+1}, \tag{63}$$

$$_kA_{k+1} = (n-1)n^{-1}\lambda_k + n^{-1}\lambda_{k+1} \tag{64}$$

never happen simultaneously.

Combining several of our results we have Theorem 9.

THEOREM 9. *In the linear inequalities the maximum number of equality signs that can appear for a given* U *is two.*

PROOF. If more than two equality signs appeared in the set of linear inequalities, there would have to be a pair of the types (61), (62), or a pair of the types (63), (64). This shows the maximum number of equality signs for any given U is ≤ 2. Theorem 6 shows that for any given H we can achieve two equality signs for an appropriate U. In particular we can always achieve $_{n-1}A_n = (n-1)n^{-1}\lambda_n + n^{-1}\lambda_{n-1}$ and $_1A_2 = (n-1)n^{-1}\lambda_1 + n^{-1}\lambda_2$ simultaneously.

This completes our discussion of simultaneous equalities in the linear inequalities.

5. Conditions Under Which Each $_{j-1}A_j$ Covers Its Full Interval of Permissible Values as U Varies

In section 5 we do not require that $\lambda_1, \ldots, \lambda_n$ be distinct. The linear inequalities (2) are valid for matrices with nondistinct eigenvalues.

THEOREM 10. *Suppose that, as* U *varies over all unitary matrices, each interval*

$$[(n-1)n^{-1}\lambda_{j-1} + n^{-1}\lambda_j,\ n^{-1}\lambda_{j-1} + (n-1)n^{-1}\lambda_j]$$

is completely filled out by $_{j-1}A_j$, $j = 2, 3, \ldots, n$. *Then*

(i) H *is scalar; or*

(ii) H *has eigenvalues* $a + b\gamma_i$, $i = 1, 2, \ldots, n$, a, b *real constants, where* $\gamma_1, \gamma_2, \ldots, \gamma_n$ *are the roots of the polynomial*

$$(\lambda^2 - 1)\frac{d}{d\lambda}P_{n-1}(\lambda).$$

Here $P_{n-1}(\lambda)$ *is the Legendre polynomial of degree* $n-1$. *Conversely, in each of Case* (i), *Case* (ii), *each interval* (65) *is completely covered by* $_{j-1}A_j$ *as* U *varies over all unitary matrices,* $j = 2, 3, \ldots, n$.

PROOF. If $H = \gamma I$ is scalar then each interval (65) consists of the single point γ and each $_{j-1}A_j = \gamma$, hence the result is trivial in Case (i). Suppose H has at least two distinct eigenvalues. Let $\mu_1 < \mu_2 < \ldots < \mu_s$ with multiplicities $e_1, e_2, \ldots, e_s$ be the distinct eigenvalues of H. We now use the notation of [1]. By [1, (19) and (20)],

$$\theta_{i\alpha} \leq (\mu_\alpha - \xi_{i,\alpha-1})/(\mu_\alpha - \mu_{\alpha-1}), \qquad \alpha \neq 1,$$

$$\theta_{i\alpha} \leq (\xi_{i\alpha} - \mu_\alpha)/(\mu_{\alpha+1} - \mu_\alpha), \qquad \alpha \neq n,$$

and $\Sigma_{i=1}^{p}\theta_{i\alpha}=e_\alpha$. Thus by summation we get stronger linear inequalities:

$$_{\alpha-1}A_\alpha \leqslant (n-e_\alpha)n^{-1}\mu_\alpha + e_\alpha n^{-1}\mu_{\alpha-1}, \qquad \alpha \neq 1, \tag{66}$$

$$_{\alpha}A_{\alpha+1} \geqslant (n-e_\alpha)n^{-1}\mu_\alpha + e_\alpha n^{-1}\mu_{\alpha+1}, \qquad \alpha \neq n. \tag{67}$$

Now if the full interval (65) is covered by $_{j-1}A_j$ for each j, then for some U we achieve

$$_{\alpha-1}A_\alpha = (n-1)n^{-1}\mu_\alpha + n^{-1}\mu_{\alpha-1}, \qquad \alpha \neq 1 \tag{68}$$

and for some other U we get

$$_{\alpha}A_{\alpha+1} = (n-1)n^{-1}\mu_\alpha + n^{-1}\mu_{\alpha+1}, \qquad \alpha \neq n. \tag{69}$$

Combining (66) and (68) yields $(e_\alpha - 1)\mu_\alpha \leqslant (e_\alpha - 1)\mu_{\alpha-1}$, a contradiction unless $e_\alpha = 1$. Combining (67) and (69) yields $(e_\alpha - 1)\mu_{\alpha+1} \leqslant (e_\alpha - 1)\mu_\alpha$, again a contradiction except if $e_\alpha = 1$. Thus $e_\alpha = 1$ for every α. That is, the eigenvalues of H are simple.

Now we are in a position to apply the results of section 4. In the present situation back to back equalities of the type described in Theorem 4 are possible, hence $f''(\lambda_j)=0$ for all $j \neq 1, n$. Thus

$$(\lambda-\lambda_1)(\lambda-\lambda_n)f''(\lambda) = n(n-1)f(\lambda). \tag{70}$$

After translation and change of scale to bring the points λ_1, λ_n to -1, 1 respectively, the differential equation (70) becomes

$$(\lambda^2-1)f''(\lambda) = n(n-1)f(\lambda). \tag{71}$$

From (71) λ^2-1 is clearly a factor of $f(\lambda)$ so put $f(\lambda)=(\lambda^2-1)g(\lambda)$. Then the differential equation for $g(\lambda)$ is

$$(1-\lambda^2)g''(\lambda) - 4\lambda g'(\lambda) + (n-2)(n+1)g(\lambda) = 0. \tag{72}$$

The differential equation for the Legendre polynomial $P_{n-1}(\lambda)$ is

$$(1-\lambda^2)P''_{n-1} - 2\lambda P'_{n-1} + (n-1)nP_{n-1} = 0 \tag{73}$$

and one easily deduces from (73) that if $g=P'_{n-1}$, then g satisfies (72). Moreover, by method of Frobenius, (72) has a unique (up to constant factor) polynomial solution. Returning to our original f, it follows that (ii) holds. For the converse when H has eigenvalues as described in (ii), we have

$$(\lambda-\lambda_1)(\lambda-\lambda_n)f''(\lambda) = n(n-1)f(\lambda)$$

and hence $f''(\lambda_j)=0$ for all $j \neq 1, n$. Then Theorems 4 or 5 show that each $_{j-1}A_j$ covers its full interval of permissible values.

6. References

[1] R. C. Thompson, Principal submatrices of normal and Hermitian matrices, Illinois J. Math. **10**, 296–308 (1966).

[2] R. C. Thompson and P. McEnteggert, Principal submatrices II: The upper and lower quadratic inequalities, to appear.

(Paper 72B1–254)

JOURNAL OF RESEARCH of the National Bureau of Standards—B. Mathematical Sciences
Vol. 72B, No. 1, January–March 1968

The Diophantine Equation $P(x, y) = (xy + d)z$

Charles F. Osgood

Institute for Basic Standards, National Bureau of Standards, Washington, D.C. 20234

(January 9, 1968)

Under certain conditions the algebraic equation $P(x, y) = (xy+d)z$, where $P(x, y)$ is a polynomial in x and y with integral coefficients and d is an integer, is shown to have an infinite number of distinct solutions with x, y, and z each an integer

Key Words: Algebraic equations, diophantine equations, integers, three variables.

L. J. Mordell[1] suggested the problem of finding solutions of the diophantine equation

$$ax^3 + by^3 + c = z(xy + d)$$

where a, b, c, and d are integers. We shall prove below that under certain conditions the equation

$$P(x, y) = z(xy + d)$$

has an infinite number of solutions, where $P(x, y)$ denotes a polynomial in x and y with integral coefficients.

We may write $P(x, y) \equiv P_1(x) + P_2(y) \mod (xy+d)$ and suppose that $P_2(0) = 0$. It is easily verified that this representation is unique. Suppose now that (a) $\deg P_1(x) + \deg P_2(y) \geq 4$, (b) $\alpha = \deg P_2(y) \geq \max(\deg P_1(x), 3)$, (c) $d \neq 0$, and (d) that $(P_1(t), d) = 1$ whenever $(t, d) = 1$. Additionally, where $P_2(y) = \beta_0 y^\alpha + \beta_1 y^{\alpha-1} + \ldots$, we suppose that (e) $\beta_0 | \beta_1^k$ for some $k \geq 1$. Under these conditions we shall prove:

THEOREM. *The diophantine equation*

$$P(x, y) = z(xy + d)$$

has an infinite number of distinct solutions.

PROOF: The genesis of the following proof was the rather trivial remark that if x and y are chosen such that $xy = 1 - d$ then $(x, y, ax^3 + by^3 + c)$ is a solution of our equation. This gives only a finite number of solutions; however, we are able to show that if $|d| > 1$ then there is almost a 1–1 correspondence of solutions between our equation and each of an infinite collection of equations of the same general type, where the number of divisors of the integer corresponding to $1 - d$ is *not uniformly bounded.* (Note $d = 0$ is contrary to the hypotheses. If $d = \pm 1$, $\{(0, y, \pm P(0, y))\}$ is an infinite collection of distinct solutions. Therefore we assume $|d| > 1$ in what follows.)

We must show that if $|d| > 1$

$$P_1(x) + P_2(y) = z(xy + d) \tag{1}$$

[1] L. J. Mordell, The congruence $ax^3 + by^3 + c \equiv 0 \pmod{xy}$ and integer solutions of cubic equations in three variables, Acta Math. **88**, 77–83 (1922).

has an infinite number of solutions. Now (1) is implied by

$$x^{\alpha}(P_1(x)+P_2(y))=z'(xy+d), \tag{2}$$

where $(xy, d)=1$. We may reduce $x^{\alpha}(P_1(x)+P_2(y))$ modulo $xy+d$ to obtain

$$R(x)=a_nx^n+\ldots+a_jx^j\ \ldots+a_3x^3+a_2dx^2+a_1d^2x+a_0d^3,$$

for integers $a_n, \ldots, a_0$ with $n\geq 4$, $a_n\neq 0$, and $a_0\neq 0$. (Recall that $\deg P_1(x)+\deg P_2(x)\geq 4$ and $\alpha=\deg P_2(y)\geq 3$.) Also $a_0|a_1^k$ for some $k\geq 1$. This means (1) is implied by

$$R(x)=z''(xy+d), \tag{3}$$

where $(xy, d)=1$. Since $x^{\alpha}(P_1(x)+P_2(y))\equiv R(x) \bmod (xy+d)$ we have, setting $y=0$,

$$R(x)\equiv x^{\alpha}(P_1(x)) \bmod d.$$

Hence if $(xy, d)=1$ then $(R(x), d)=1$ by hypothesis (d).

If (3) has an infinite number of solutions with $(xy, d)=1$ then (1) has an infinite number of solutions. For technical reasons we shall find it easier to show that

$$y_1^n-a_1dy_1^{n-1}+a_2(a_0d^2)y_1^{n-2}+a_3a_0d(-a_0d^2)y_1^{n-3}+\ldots+a_ja_0d(-a_0d^2)^{j-2}$$

$$y_1^{n-j}+\ldots+a_na_0d(-a_0d^2)^{n-2}=w_4(x_1y_1-a_na_0d(-a_0d^2)^{n-3}), \tag{4}$$

with $(x_1y_1, a_na_0d)=1$, has an infinite number of solutions. Hence we must show that (4) having an infinite number of solutions implies that (3) has an infinite number of solutions. Looking at (4) mod y_1 we see that it implies, setting $w_4=xy_1+a_0d^2$ and $(x_1y_1-a_na_0d(-a_0d^2)^{n-3})=w_3$ that we have

$$y_1^n-a_1dy_1^{n-1}+a_2(a_0d^2)y_1^{n-2}+a_3a_0d(-a_0d^2)y_1^{n-3}+\ldots+a_ja_0d(-a_0d^2)^{j-2}$$

$$y_1^{n-j}+\ldots+a_n(a_0d)(-a_0d^2)^{n-2}=w_3(xy_1+a_0d^2). \tag{5}$$

Now $(y_1, a_0d)=1$ so $(y_1-a_1d, a_0d)=1$ (use $a_0|a_1^k$ for some k), and $(xy_1, a_0d)=1$. We note that

$$(y_1, x, w_3)=\left(y_1, \frac{w_4-a_0d^2}{y_1}, x_1y_1-a_na_0d(-a_0d^2)^{n-3}\right)$$

so distinct solutions go into distinct solutions. It follows that (5) implies, setting $w_2=a_0d^3w_3$, that

$$a_n(-a_0d^2)^n+\ldots+a_j(-a_0d^2)^jy_1^{n-j}+\ldots+a_3(-a_0d^2)^3y_1^{n-3}$$

$$+a_2d(-a_0d^2)^2y_1^{n-2}+a_1d^2(-a_0d^2)y_1^{n-1}+a_0d^3y_1^n=w_2(xy_1+a_0d^2) \tag{6}$$

where

$$(xy_1, a_0d)=1.$$

Now (6) implies, setting $w_1=w_2y_1^{-n}$, that

$$R(x)=a_nx^n+\ldots+a_jx^j+\ldots+a_3x^3+a_2dx^2+a_1d^2x+a_0d^3=w_1(xy_1+a_0d^2). \tag{7}$$

We conclude that (7) implies, setting $w_1 = (xy+d)$ and $(xy_1 + a_0d^2) = z''$, that

$$R(x) = z''(xy+d). \tag{3}$$

Since $(x, d) = 1$ we have $(R(x), d) = 1$, so $(xy, d) = 1$. In this last change of variables (x, y_1, w_1) becomes

$$\left(x, \frac{z_1'' - a_0d^2}{x}, xy+d\right)$$

so distinct solutions go into distinct solutions.

Now to show that (4) has an infinite number of solutions. We shall show that there exists an infinite sequence of equations $E_0, E_2, \ldots$ with $E_0 = (4)$ and $E_{2i} \leftrightarrow E_{2i+2}$ in the sense that a sequence of *reversible* steps takes one equation into the other—inducing a 1–1 correspondence of solutions. Then we shall end with a proof that given $N > 0$ there exists an n such that E_{2n} has at least N distinct solutions.

DEFINITION: *Let* $\beta(\mathrm{m})$ *be a function from the integers to the integers defined by* $\beta(0) = 0, \beta(1) = 1$, *and*

$$\beta(\mathrm{m}) = (\mathrm{n}-2)\beta(\mathrm{m}-1) - \beta(\mathrm{m}-2).$$

Notice that since $\mathrm{n} \geq 4$ *if* $\mathrm{s}(\mathrm{m})$ *satisfies the above recurrence relation and* $0 \leq \mathrm{s}(0) \leq \mathrm{s}(1)$ *then* $\mathrm{s}(\mathrm{m})$ *is nondecreasing for all* $\mathrm{m} \geq 0$. *Therefore* $\beta(\mathrm{m}+1) - \beta(\mathrm{m})$ *is nondecreasing for all* $\mathrm{m} \geq 0$.

DEFINITION: *For each integer* m *set*

$$\mathrm{r_m} = (-1)^{\beta(\mathrm{m}+1)+1}(\mathrm{a_n d^{-1}})^{\beta(\mathrm{m}+1)}(-\mathrm{a_0 d^2})^{\beta(\mathrm{m}+2)} \equiv (-1)^{\beta(\mathrm{m}+1)+1}(-\mathrm{a_n a_0 d}(-\mathrm{a_0 d^2})^{n-4})^{\beta(\mathrm{m}+1)}(-\mathrm{a_0 d^2})^{\beta(\mathrm{m}+1)-\beta(\mathrm{m})},$$

using $\beta(\mathrm{m}+2) = (\mathrm{n}-4)\beta(\mathrm{m}+1) + \beta(\mathrm{m}+1) + \beta(\mathrm{m}+1) - \beta(\mathrm{m})$. *From the second expression for* $\mathrm{r_m}$ *we are able to conclude that if* $\mathrm{m} \geq 0$ *then* $(\mathrm{a_n a_0 d})^{-1}(\mathrm{r_m})^{-1}\mathrm{r_{m+1}}$ *is an integer by using the facts that* $\beta(\mathrm{m}+2) - \beta(\mathrm{m}+1)$ *is nondecreasing if* $\mathrm{m} \geq -1$, *and* $\beta(1) - \beta(0) = 1$.

Now write (4) as

$$\sum_{k=0}^{n} A_k^0 y^k = z''(xy + r_0)$$

which defines A_k^0 for each $0 \leq k \leq n$. In what follows we assume $m \geq 0$. Let

$$A_k^{2m} = A_k^0 \prod_{j=1}^{m} (r_{2j-1}r_{2j-2}^{-1})^{n-k}. \tag{8}$$

Then $|A_k^{2m}|$ is a power product of a_0, a_n, and d. By our remarks above $(a_n a_0 d)^{-1}A_k^{2m}$ is an integer if $0 \leq k < n$.

Using (8) we derive the result that for each $0 \leq k \leq n$

$$(r_{2m})^k A_k^{2m}(A_0^{2m})^{-1} = \left\{\prod_{j=1}^{m} (r_{2j}r_{2j-1}^{-1})^k\right\} r_0^k A_k^0 (A_0^0)^{-1}. \tag{9}$$

Checking (4), we see that $r_0^k A_k^0 (A_0^0)^{-1}$ is always an integer, hence so is the left side of (9). If $0 < k \leq n$, $(a_0 a_n d)^{-1} r_{2m}^k A_k^{2m}(A_0^{2m})^{-1}$ is an integer by the remark after the definition of r_m. We need to show that

$$r_{2m+1} = (-1)^n (A_0^{2m})^{-1}(r_{2m})^{n-1}. \tag{10}$$

Using (9) with $k = n$ we see that the right-hand side of (10) is

$$(-1)^n (A_0^0)^{-1} r_0^n r_{2m}^{-1} \left\{\prod_{j=1}^{m} (r_{2j}r_{2j-1}^{-1})^n\right\}.$$

Using the definition of r_m, we compare the exponents on r_0, $a_n d^{-1}$, and $-a_0 d^2$, and observe that

$$n\sum_{j=1}^{m}\{\beta(2j+1)-\beta(2j)\}=\sum_{j=1}^{m}\{\beta(2j+2)+2\beta(2j+1)+\beta(2j)-\beta(2j+1)-2\beta(2j)-\beta(2j-1)\}$$

$$=\beta(2m+2)+\beta(2m+1)-\beta(2)-\beta(1)=\gamma(2m+2)-\gamma(2) \text{ where } \gamma(m)=\beta(m)+\beta(m-1).$$

It follows that

$$r_0^n(a_n d^{-1})^{\gamma(2m+2)-\gamma(2)}(-a_0 d^2)^{\gamma(2m+3)-\gamma(3)}(-1)^{\gamma(2m+2)-\gamma(2)+n}=A_0^0 r_{2m}r_{2m+1}.$$

Using the first expression for r_{2m} we see that this is equivalent to

$$(-1)^n r_0^{n-1}r_1^{-1}=A_0^0 \tag{11}$$

or

$$-(-a_n a_0 d(-a_0 d^2)^{n-4})^{n-1}\cdot((-a_n a_0 d(-a_0 d^2)^{n-4})^{-(n-2)}(-a_0 d^2)^2)=a_n a_0 d(-a_0 d^2)^{n-2}=A_0^0,$$

which may be verified from (4).

We must also establish

$$r_{2m+2}=A_0^{2m}(r_{2m+1})^{n-1}(r_{2m})^{-n}. \tag{12}$$

This is equivalent to

$$r_{2m+2}r_{2m+1}=(r_{2m+1}r_{2m}^{-1})^n A_0^{2m}.$$

By (8) we must prove that

$$r_{2m+2}r_{2m+1}=A_0^0\prod_{j=1}^{m+1}(r_{2j-1}r_{2j-2}^{-1})^n.$$

Summing exponents again we have

$$r_{2m+2}r_{2m+1}=A_0^0(-a_n d^{-1})^{\gamma(2m+3)-\gamma(1)}(-a_0 d^2)^{\gamma(2m+4)-\gamma(2)}$$

$$=A_0^0 r_{2m+2}r_{2m+1}(-a_n d^{-1})^{-\gamma(1)}(-a_0 d^2)^{-\gamma(2)}=A_0^0 r_{2m+2}r_{2m+1}(r_0 r_{-1})^{-1},$$

using the recursion formula for $\beta(m)$ and the formula for r_m. We see that (12) is equivalent to

$$A_0^0=r_0 r_{-1}=(-1)^n r_0^{n-1}r_1^{-1},$$

which is (11).

We verify that

$$A_k^{2m}(-r_{2m})^k(-r_{2m+1})^{n-k}((-r_{2m})^n)^{-1}=A_k^{2m}(r_{2m+1}r_{2m}^{-1})^{n-k}=A_k^{2m+2}, \tag{13}$$

using the definition of A_k^{2m+2}.

Set $k=0$ in (13). Then using $A_0^{2m+2}=A_0^{2m}(r_{2m+1}r_{2m}^{-1})^n$ along with (12) we may write

$$r_{2m+2}=A_0^{2m+2}(r_{2m+1})^{-1}. \tag{14}$$

We define E_{2m} to be the equation

$$\sum_{k=0}^{n} A_k^{2m}x^k=v_1(xy+r_{2m}), \tag{15}$$

where $$(xy,\ a_0a_nd)=1.$$

Now $E_0=(4)$. By induction we shall show that for each $m\geq 0$ E_{2m+2} is equivalent to E_{2m}. Line (15) is equivalent to

$$\sum_{k=0}^{n} A_k^{2m}x^ky^n=v_2(xy+r_{2m}) \text{ with } (xy,\ a_0a_nd)=1. \tag{16}$$

(Recall that r_m is a power product of a_0, a_n, and d which is divisible by a_0a_nd, for each $m\geq 0$.)

Line (16) is equivalent to

$$\sum_{k=0}^{n} A_k^{2m}(-r_{2m})^ky^{n-k}=v_3(xy+r_{2m}), \text{ with } (xy,\ a_0a_nd)=1. \tag{17}$$

Now (17) is equivalent to

$$\sum_{k=0}^{n} A_k^{2m}(A_0^{2m})^{-1}(-r_{2m})^ky^{n-k}=v_4(xy+r_{2m}), \text{ with } (xy,\ a_0a_nd)=1 \tag{18}$$

by the comment after (9) and the fact that $|A_0^{2m}|$ is a power product of a_0, a_n, and d. Taking both sides of (18) mod y and using $(y,\ a_0a_nd)=\overline{1}$ we see that

$$v_4=x_1y+(A_0^{2m})^{-1}(-r_{2m})^n(r_{2m})^{-1}=x_1y+r_{2m+1}$$

by (10). Since a_0a_nd divides $A_k^{2m}(A_0^{2m})^{-1}(-r_{2m})^k$ if $k>0$ (see the comment after line (9)) we see that $(x_1y,\ a_0a_nd)=1$. Using (10) we may write the equivalent statement

$$\sum_{k=0}^{n} A_k^{2m}(A_0^{2m})^{-1}(-r_{2m})^ky^{n-k}=v_5(x_1y+r_{2m+1}), \text{ with } (x_1y,\ a_0a_nd)=1. \tag{19}$$

As before we may write

$$\sum_{k=0}^{n} A_k^{2m}(A_0^{2m})^{-1}(-r_{2m})^ky^{n-k}x_1^n=v_6(x_1y+r_{2m+1}), \text{ with } (x_1y,\ a_0a_nd)=1, \tag{20}$$

instead of (19), so

$$\sum_{k=0}^{n} A_k^{2m}(A_0^{2m})^{-1}(-r_{2m})^k(-r_{2m+1})^{n-k}x_1^k=v_7(x_1y+r_{2m+1}) \text{ with } (x_1y,\ a_0a_nd)=1 \tag{21}$$

is also equivalent to (19). We may write, after dividing above by $(A_0^{2m})^{-1}(-r_{2m})^n$, the equivalent statement

$$\sum_{k=0}^{n} A_k^{2m+2}x_1^k=v_8(x_1y+r_{2m+1}), \text{ with } (x_1y,\ a_0a_nd)=1, \tag{22}$$

by (13) and the fact that $(A_0^{2m})^{-1}(-r_{2m})^n$ is a power product of a_0, a_n, and d. Taking (22) mod x_1 we see that

$$v_8 = x_1y_1 + A_0^{2m+2}(r_{2m+1})^{-1} = x_1y_1 + r_{2m+2}, \text{ by (14), where } (x_1y_1,\ a_0a_nd) = 1$$

by the remark after (8). Thus (15) is equivalent to

$$\sum_{k=0}^{n} A_k^{2m+2}x_1^k = v_9(x_1y_1 + r_{2m+2}). \tag{23}$$

This completes the induction.

Now to find solutions of

$$\sum_{k=0}^{n} A_k^{2m}x^n = v_1(xy + r_{2m}). \tag{24}$$

Suppose we solve $xy + r_{2m} = 1$. Obviously (24) has solutions corresponding to these choices of x and y.

Set $a_na_0d(-a_0d^2)^{n-4} = A$ and $-a_0d^2 = B$. Note $|A| > 1$ and $|B| > 1$, as $|d| > 1$. If

$$xy = A^{\beta(2m+1)}B^{\beta(2m+1)-\beta(2m)} + 1 = 1 - r_{2m}$$

we have a solution of E_{2m}. Given $N > 0$ we shall show that we may choose m such that $1 - r_{2m}$ has at least N distinct pairs of factors. (Then E_{2m} has at least N solutions as does the original equation.)

Let w and $\overline{w}$ be the roots of $x^2 - (n-2)x + 1 = 0$. Note that w is a unit in the ring R of algebraic integers in $Q(\sqrt{n^2-4n})$. Thus for any rational integer $k > 1$, w, and $\overline{w}$ go into units when we form the ring R/kR. The units in R/kR form a finite group so there exists a positive integer θ such that $(\omega)^\theta \equiv 1 \bmod kR$. Using the formula for $\beta(m)$ from finite differences, we see that

$$\beta(2m + 2\theta + 1) \equiv \beta(2m + 1) \bmod kR$$

and

$$\beta(2m + 2\theta) \equiv \beta(2m) \bmod kR;$$

clearly both congruences hold also mod k. Setting $k = \varphi(|1 - r_0|)$ it follows that $1 - r_0$ divides $1 - r_{2\theta}$. Now set $k_1 = \varphi(|1 - r_{2\theta}|)$, and continue. (Note that as $|A| > 1$ and $|B| > 1$ the $|1 - r_{2m}|$ form an increasing sequence.) We see that the number of factors of $1 - r_{2m}$ goes to infinity on a subsequence of positive integers m. This concludes the proof of the Theorem.

(Paper 72B1–255)

JOURNAL OF RESEARCH of the National Bureau of Standards – B. Mathematical Sciences
Vol. 72B, No. 1, January–March 1968

A Note on the G-Transformation*

H. L. Gray and T. A. Atchison****

(December 12, 1967)

Recent literature concerning the use of nonlinear transformations to evaluate numerically certain improper integrals of the first kind has shown that difficulties are encountered if the integrand f is such that

$$\lim_{t\to\infty}\frac{f(t+k)}{f(t)}=1.$$

This note introduces a new nonlinear transformation which is in some cases quite useful when the above limit is one. A simple example is given to illustrate the use of this transformation.

Key Words: Improper integrals, nonlinear transformations.

1. Introduction

In a recent paper [1],[1] H. L. Gray and T. A. Atchison have introduced a nonlinear transformation for the purpose of evaluating improper integrals of the first kind. This transformation is most useful on integrals of the type

$$\int_a^\infty f(x)dx, \tag{1.1}$$

where

$$\lim_{t\to\infty}\frac{f(t+k)}{f(t)}=R\neq 0 \text{ or } 1. \tag{1.2}$$

In this note, a new transformation is introduced which will be more suitable when $R=1$ and which reduces to the transformation defined in [1] when $R\neq 1$.

2. The Transformation

Let

$$F(t)=\int_a^t f(x)dx\to S \text{ as } t\to\infty. \tag{2.1}$$

When the following limit exits, let

$$\alpha=\lim_{t\to\infty}\frac{1-R(t;\,k)}{R(t;\,k)}\,\frac{E(t+k)}{F(t+k)-F(t)} \tag{2.2}$$

where $R(t;\,k)=f(t+k)/f(t)$ and $E(t+k)=S-F(t+k)$.

---

*An invited paper.

**Present address: Texas Technological College, Department of Mathematics, P.O. Box 4319, Lubbock, Texas 79409.

[1] H. L. Gray and T. A. Atchison. Nonlinear transformations related to the evaluation of certain improper integrals, SIAM Journal on Numerical Analysis 4, No. 3, 363–371 (1967).

DEFINITION 2.1. *Let*

$$L[F;\ t,\ k]=F(t+k)+\alpha R(t;\ k)\,\frac{F(t+k)-F(t)}{1-R(t;\ k)}, \tag{2.3}$$

where we assume α exists and $R(t;\ k)\neq 1$.

In order to determine α from (2.2), the value of the integral S appears to be necessary. The following considerations show that this is not always true. Note that

$$\frac{1-R(t;\ k)}{R(t;\ k)}\,\frac{E(t+k)}{F(t+k)-F(t)}=\frac{E(t+k)/[1/f(t+k)-1/f(t)]^{-1}}{[F(t+k)-F(t)]/f(t)}. \tag{2.4}$$

If $1/f(t+k)-1/f(t)\to\infty$ as $t\to\infty$, then L'Hospital's rule can be applied to the numerator and denominator separately to assist in determining α. That is, if the limits exist and the denominator limit is not zero,

$$\alpha=\frac{\lim\limits_{t\to\infty}-f(t+k)/\ \dfrac{d}{dt}\,[1/f(t+k)-1/f(t)]^{-1}}{\lim\limits_{t\to\infty}\ [f(t+k)-f(t)]/f'(t)}. \tag{2.5}$$

Note that (2.5) does not involve any integration.

THEOREM 2.1. $L[F;\ t,\ k]\to S$ *as* $t\to\infty$ *if, and only if,*

$$\alpha\ \lim_{t\to\infty} R(t;\ k)\,\frac{F(t+k)-F(t)}{1-R(t;\ k)}=0. \tag{2.6}$$

PROOF. This follows immediately from Definition 2.1.

THEOREM 2.2. $L[F;\ t,\ k]\to S$ *as* $t\to\infty$.

PROOF. If $\alpha=0$, the result is immediate from Theorem 2.1.

If $\alpha\neq 0$, then

$$\alpha\lim_{t\to\infty} R(t;\ k)\,\frac{F(t+k)-F(t)}{1-R(t;\ k)}=\lim_{t\to\infty} E(t+k)=0 \tag{2.7}$$

and the result follows from Theorem 2.1.

The fact that $L[F;\ t,\ k]$ converges to S is of importance. However, the purpose of this transformation is to obtain a function which converges to S more rapidly than the original integral.

THEOREM 2.3. *If* $\alpha\neq 0$, *then* $L[F;\ t,\ k]\to S$ *more rapidly than* $F(t+k)$ *as* $t\to\infty$.

PROOF. Since

$$\begin{aligned}\frac{S-L[F;\ t,\ k]}{S-F(t+k)}&=\frac{S-F(t+k)-\alpha R(t;\ k)\,\dfrac{F(t+k)-F(t)}{1-R(t;\ k)}}{S-F(t+k)}\\ &=1-\alpha\,\frac{R(t;\ k)}{1-R(t;\ k)}\,\frac{F(t+k)-F(t)}{E(t+k)}\end{aligned} \tag{2.8}$$

and $\alpha\neq 0$, then

$$\lim_{t\to\infty}\frac{S-L[F;\ t,\ k]}{S-F(t+k)}=1-\alpha\,\frac{1}{\alpha}=0. \tag{2.9}$$

Note that if $\alpha=0$, then $L[F;\ t,\ k]=F(t+k)$ and more rapid convergence is not achieved. Another interesting relation occurs if $\alpha=1$. In this case $L[F;\ t,\ k]=G[F;\ t,\ k]$, the nonlinear transformation introduced in [1]. The circumstances under which L will reduce to G are considered in the next theorem.

THEOREM 2.4. *If* $\lim_{t\to\infty} R(t; k) = R(k) \neq 0, 1,$ *then* $L[F, t, k] = G[F; t, k]$.
PROOF. Since

$$\lim_{t\to\infty} \frac{E(t+k)}{F(t+k)-F(t)} = \lim_{t\to\infty} \frac{-f(t+k)}{f(t+k)-f(t)}$$

$$= \lim_{t\to\infty} \frac{R(t; k)}{1-R(t; k)} = \frac{R(k)}{1-R(k)}, \tag{2.10}$$

then $\alpha = 1$ and the theorem follows.

The importance of the transformation L lies in the fact that regardless of the limit of $R(t; k)$, if α exists and is different from zero, then more rapid convergence to S is still achieved. This is best illustrated by considering the following simple example in which $G[F; t, k]$ fails to converge more rapidly than $F(t+k)$ but $L[F; t, k]$ converges more rapidly than $G[F; t, k]$ or $F(t+k)$.

Let $f(x) = 1/(1+x^2)$. Then

$$R(t; k) = \frac{1+t^2}{1+(t+k)^2} \to 1 \text{ as } t \to \infty. \tag{2.11}$$

However,

$$\alpha = \lim_{t\to\infty} \frac{(2kt+k^2)\int_{t+k}^{\infty} \frac{1}{1+x^2}\,dx}{(1+t^2)\int_{t}^{t+k} \frac{1}{1+x^2}\,dx} = \frac{2k}{k} = 2 \tag{2.12}$$

as may be determined by using eq (2.5). The transformation described in this paper becomes

$$L[F; t, k] = \int_0^{t+k} \frac{1}{1+x^2}\,dx + 2\frac{1+t^2}{2kt+k^2}\int_t^{t+k} \frac{1}{1+x^2}\,dx. \tag{2.13}$$

Taking $t = 20$ and $k = 0.1$,

$$L[F; 20, 0.1] \simeq 1.571213756 \tag{2.14}$$

which is in error by about 0.0004. It should be noted that arc tan 20.1 is in error by about 0.05 while $G[F; 20, 0.1]$ is in error by approximately 0.02.

Clearly the integral above, being very simple, could be integrated quite satisfactorily by a number of other numerical methods.-However it adequately illustrates the comparison between L and G.

(Paper 72B1–256)

289-930 OL-68—3

JOURNAL OF RESEARCH of the National Bureau of Standards—B. Mathematical Sciences
Vol. 72B, No. 1, January–March 1968

The Distribution of the Sample Correlation Coefficient With One Variable Fixed

David Hogben

Institute for Basic Standards, National Bureau of Standards, Washington, D.C. 20234

(November 30, 1967)

For the usual straight-line model, in which the independent variable takes on a fixed, known set of values, it is shown that the sample correlation coefficient is distributed as Q with $(n-2)$ degrees of freedom and noncentrality $\theta=(\beta/\sigma)\sqrt{\Sigma(x_i-\bar{x})^2}$. The Q variate has been defined and studied elsewhere by Hogben et al. It is noted that the square of the correlation coefficient is distributed as a noncentral beta variable.

Key Words: Analysis of variance, calibration, correlation coefficient, degrees of freedom, distribution, fixed variable, noncentral beta variable, noncentrality, Q variate.

1. Introduction

Consider the straight-line model

$$Y_i=\alpha+\beta x_i+\epsilon_i, \qquad i=1, 2, \ldots, n \tag{1}$$

where

(i) the ϵ_i are assumed to behave as normally and independently distributed random variables with mean zero and common variance σ^2,

(ii) α and β are unknown parameters, and

(iii) lowercase italic letters denote fixed, known constants and uppercase italic letters denote random variables, i.e., x is fixed and Y is random. This and other straight-line models are discussed in detail by Acton [1959].

The sample correlation coefficient r_{xY} is defined by

$$r_{xY}=\frac{\sum_{i=1}^{n}(x_i-\bar{x})(Y_i-\bar{Y})}{\sqrt{\sum_{i=1}^{n}(x_i-\bar{x})^2\sum_{i=1}^{n}(Y_i-\bar{Y})^2}}, \tag{2}$$

where $$\bar{x}=\sum_{i-1}^{n}x_i/n \text{ and } \bar{Y}=\sum_{i-1}^{n}Y_i/n.$$

It is of some interest in the calibration problem where a fitted straight-line is used in reverse for estimating an unknown x_0 corresponding to an observed Y_0. The distribution of r_{XY} where X and Y follow the bivariate normal is well known; see for example Kendall and Stuart [1961, pp. 383–390]. In the present paper the distribution of r_{xY} as defined by (2) is derived for x fixed. This distribution

is well known for the special case with all Y_i identically distributed (i.e., $\beta = 0$), in which case it is the same as the distribution of r_{XY} for X, Y independent and normal. See, e.g., Hotelling [1953, p. 196]. J. N. K. Rao and an unidentified person have pointed out that the distribution of r^2_{xY} can be obtained as a special case of the conditional distribution of the multiple correlation coefficient for the multi-variate normal; see, e.g., C. R. Rao [1965, p. 509].

2. Derivation

In an analysis of variance for the model (1) the (corrected) total sum of squares with $(n-1)$ degrees of freedom may be partitioned into two independent components; the first being the sum of squares due to the slope with 1 degree of freedom and the second being the residual sum of squares with $(n-2)$ degrees of freedom. This partition can be expressed by

$$\sum_{i=1}^{n} (Y_i - \overline{Y})^2 = \frac{\left[\sum (x_i - \overline{x})(Y_i - \overline{Y})\right]^2}{\sum (x_i - \overline{x})^2} + \sum (Y_i - \hat{Y}_i)^2, \tag{3}$$

where

$$\hat{Y}_i = \overline{Y} + \hat{\beta}(x_i - \overline{x})$$

and

$$\hat{\beta} = \sum_{i-1}^{n} (x_i - \overline{x})(Y_i - \overline{Y}) \Big/ \sum_{i-1}^{n} (x_i - \overline{x})^2$$

is the usual least squares estimator for β. Let the random variables W and X^2 be defined by

$$W = \frac{\sum (x_i - \overline{x})(Y_i - \overline{Y})}{\sigma \sqrt{\sum (x_i - \overline{x})^2}}, \tag{4}$$

and

$$X^2 = \sum (Y_i - \hat{Y}_i)^2 / \sigma^2. \tag{5}$$

Using (4) and (5) and dividing both sides of eq (3) by σ^2 we have

$$\sum_{i=1}^{n} (Y_i - \overline{Y})^2 / \sigma^2 = W^2 + X^2. \tag{6}$$

If both the numerator and denominator of r_{xY} are divided by σ^2 and the first factor of the denominator is combined with the numerator, the correlation coefficient may be written as

$$r_{xY} = \frac{W}{\sqrt{W^2 + X^2}}. \tag{7}$$

Since the Y_i are normally distributed, it is easily shown that W is normally distributed with mean $\theta = (\beta/\sigma)\sqrt{\Sigma(x_i - \overline{x})^2}$ and variance 1. Further, it is well known from the theory of the general linear hypothesis that under model (1) W and X^2 are independently distributed and X^2 is distributed as chi-squared with $(n-2)$ degrees of freedom. Therefore, r_{xY} is equal to the random variable Q defined and studied in Hogben et al., [1964a] and [1964b]. Hence, the following theorem is proved.

THEOREM: The correlation coefficient r_{xY}, defined by (2) under model (1), is distributed as Q with $(n-2)$ degrees of freedom and noncentrality $\theta = (\beta/\sigma)\sqrt{\Sigma(x_i - \overline{x})^2}$.

Various properties of Q are given in the previous two references, including analytic expressions and recurrence relations for the moments about zero, numerical values for the first four central moments and an approximation to the distribution of Q by that of a linearly transformed beta variable. It follows from (7) that r_{xY}^2 is distributed as noncentral beta; see for example Seber [1963], where in his notation $n_1=1$, $n_2=n-2$ and $\lambda=\theta^2/2$. Furthermore, $t=\sqrt{(n-2)r^2/(1-r^2)}$ is distributed as noncentral t with noncentrality θ and $(n-2)$ degrees of freedom. The distribution of r_{xY} also follows from the interesting and easily derived relation

$$r_{xY}=\frac{\hat{\beta}}{\sqrt{\hat{\beta}^2+(n-2)s_{\hat{\beta}}^2}}.$$

Thanks go to Joan Rosenblatt for pointing out the looseness of an earlier proof of the theorem and to her and Edwin L. Crow for constructive suggestions.

3. References

Acton, F. (1959), Analysis of Straight-Line Data (John Wiley & Sons, Inc., New York, N.Y.).

Hogben, D., Pinkham, R. S. and Wilk, M. B. (1964a), The moments of a variate related to the non-central t. Ann. Math. Statist., **35**, 298–314.

Hogben, D., Pinkham, R. S. and Wilk, M. B. (1964b), An approximation to the distribution of Q (a variate related to the non-central t). Ann. Math. Statist. **35**, 315–318.

Hotelling, H. (1953), New light on the correlation coefficient and its transforms. J. Roy. Statist. Soc. Ser. B, **15**, 193–225.

Kendall, M. G. and Stuart, A. (1961), The Advanced Theory of Statistics, **I.** (Hafner Publishing Co., New York).

Rao, C. R. (1965), Linear Statistical Inference and Its Application (John Wiley & Sons, Inc., New York, N.Y.).

Seber, G. A. F. (1963), The non-central chi-squared and beta distributions. Biometrika **50**, 542–544.

(Paper 72B1–257)

JOURNAL OF RESEARCH of the National Bureau of Standards—B. Mathematical Sciences
Vol. 72B, No. 1, January–March 1968

Solutions of the Time-Dependent Klein-Gordon and Dirac Equations for a Uniform Electric Field

Vernon W. Myers

Institute for Materials Research, National Bureau of Standards, Washington, D.C. 20234

(October 12, 1967)

The time-dependent Klein-Gordon and Dirac equations are solved for the motion of a charged particle in a classical uniform electrostatic field of infinite extent. The elementary solutions have a position dependence of the form $e^{i\mathbf{k}\cdot\mathbf{r}}$ with the component of k in the field direction varying linearly with time.

Key Words: Dirac and Klein-Gordon equations, time-dependent solutions, uniform electric field.

1. Introduction

Electromagnetic forces have the proper behavior under a Lorentz transformation, and this paper treats the relativistic equations for the motion of a charged particle in a uniform electrostatic field of infinite extent. The interaction of a charged particle with a quantized field is of great interest, but any thorough treatment is rather involved and necessarily requires approximations. The field will be treated classically, and such effects as polarization of the vacuum and radiation by the accelerated charge are not included. This example of a uniform electric field is chosen, because the time-dependent equations describing traveling waves can be solved in a rather straightforward manner.

It is worthwhile to examine the classical equations of motion before undertaking the quantum mechanical treatment. The uniform electrostatic field E is taken to be in the positive x direction. The gage may be chosen arbitrarily, and it does not affect any of the observables. Maxwell's equation relating E to the scalar and vector potentials is

$$\mathbf{E} = -\nabla V - \frac{1}{c}\frac{\partial \mathbf{A}}{\partial t}. \tag{1}$$

An obvious gage is $V = -Ex$, $A = 0$ for an electrostatic field $\mathbf{E} = \hat{i}E$ (E a constant). If this gage is used, the relativistic Hamiltonian for a particle of rest mass m and charge ϵ is

$$H = [m^2c^4 + c^2(p_x^2 + p_y^2 + p_z^2)]^{1/2} - \epsilon Ex. \tag{2}$$

Hamilton's equations are

$$\dot{p}_x = -\frac{\partial H}{\partial x}, \quad \dot{x} = \frac{\partial H}{\partial p_x}, \text{ etc.}$$

One finds that the various components of momentum are

$$p_x = p_{0x} + \epsilon Et, \quad p_y = p_{0y}, \quad p_z = p_{0z} \tag{3}$$

where p_{0x}, p_{0y}, p_{0z} are constants. The linear time dependence for p_x is the same as the nonrelativistic result and is due to the fact that the electric field is uniform. The traveling wave solutions of the quantum mechanical equation have the same time dependence for the momentum as the classical relations, of course.

An alternative gage is $V=0$, $\mathbf{A}=-\hat{i}cEt$. The x-component of mechanical momentum would be

$$\frac{mv_x}{\left(1-\frac{v^2}{c^2}\right)^{1/2}}=p_x-\frac{\epsilon}{c}A_x=p_x+\epsilon Et. \tag{4}$$

The Hamiltonian would be

$$H=[m^2c^4+c^2[(p_x+\epsilon Et)^2+p_y^2+p_z^2]]^{1/2} \tag{5}$$

where p_x, p_y, p_z are constants of motion. The original gage $V=-Ex$, $\mathbf{A}=0$ is preferable because p is then the mechanical momentum. In addition, the introduction of the vector potential does not simplity the solution of the quantum mechanical equations.

2. Klein-Gordon Equation

The scalar wave equation is appropriate for a spin zero particle, a charged π meson, for example. The wave equation is found by taking the classical relation

$$(H+\epsilon Ex)^2=m^2c^4+c^2p^2, \tag{6}$$

and applying it in operator form. The Klein-Gordon equation is

$$\left(i\hbar\frac{\partial}{\partial t}+\epsilon Ex\right)^2\psi=(m^2c^4-c^2\hbar^2\nabla^2)\psi. \tag{7}$$

Let

$$\psi=e^{i\mathbf{k}\cdot\mathbf{r}}T, \tag{8}$$

where k_x and T are functions of the time. The quantum mechanical expression for momentum is identical with the classical results, eq (3). That is,

$$k_x=k_{0x}+\frac{\epsilon Et}{\hbar},\quad k_y=k_{0y},\quad k_z=k_{0z} \tag{9}$$

where k_{0x}, k_{0y}, k_{0z} are constants. The linear time dependence of k_x is required if T is to be a function of the time only. The function $e^{i\mathbf{k}\cdot\mathbf{r}}$ represents a state in which the momentum and kinetic energy are known with complete certainty since it is an eigenfunction for both the momentum and kinetic energy operators.

The equation for T is found from the substitution of eq (8) into eq (7):

$$-\hbar^2\frac{d^2T}{dt^2}=[m^2c^4+c^2\hbar^2(k_x^2+k_y^2+k_z^2)]T. \tag{10}$$

In the limit of $E\rightarrow 0$, T is $e^{\pm\frac{iWt}{\hbar}}$ where W is the total energy. It is possible to find a power series solution for T. If the dimensionless quantities

$$u=\left(\frac{c\epsilon E}{\hbar}\right)^{1/2}\left(t+\frac{k_{0x}\hbar}{\epsilon E}\right)=\left(\frac{c\hbar}{\epsilon E}\right)^{1/2}k_x,$$

$$a^2=\frac{m^2c^3+c\hbar^2(k_y^2+k_z^2)}{\epsilon E\hbar} \tag{11}$$

are used, then

$$\frac{d^2T}{du^2}+(u^2+a^2)T=0. \tag{12}$$

It is interesting to note that eq (12) is the same as the nonrelativistic Schrödinger equation for the potential $-u^2$. The solution of (12) can be expressed in the following way:

$$T=\exp\left(\pm\frac{iu^2}{2}\right)\sum_0^\infty b_nu^n. \tag{13}$$

The coefficients of the series are determined by the recursion relation

$$\frac{b_{n+2}}{b_n}=\mp\frac{i(2n+1)+a^2}{(n+1)(n+2)} \tag{14}$$

for both odd and even n. The series converges for all finite values of t. The coefficients b_0 and b_1 are arbitrary. The signs in the foregoing equations are associated with positive and negative charges [1]. That is, if $e^{\frac{iu^2}{2}}$ corresponds to a positively charged meson with positive kinetic energy, then $e^{-\frac{iu^2}{2}}$ corresponds to a negatively charged meson with positive kinetic energy.

Equation (10) is very similar to the time-independent relation

$$(W+\epsilon Ex)^2\psi=(m^2c^4-c^2\hbar^2\nabla^2)\psi. \tag{15}$$

Let $\psi=e^{i(k_yy+k_zz)}\phi(x)$.
Then,

$$(W+\epsilon Ex)^2\phi=[m^2c^4+c^2\hbar^2(k_y^2+k_z^2)]\phi-c^2\hbar^2\frac{d^2\phi}{dx^2}. \tag{16}$$

Time and distance enter in a symmetrical way for this example of a uniform field.

3. Dirac Equation

The Dirac equation is for a spin ½ particle, an electron for instance. The time-dependent equation is

$$H\psi=i\hbar\frac{\partial\psi}{\partial t}. \tag{17}$$

The Dirac Hamiltonian is

$$H=-i\hbar c\left(\alpha_x\frac{\partial}{\partial x}+\alpha_y\frac{\partial}{\partial y}+\alpha_z\frac{\partial}{\partial z}\right)+\beta mc^2-\epsilon Ex. \tag{18}$$

The common representation is used:

$$\alpha_x=\begin{pmatrix}0&0&0&1\\0&0&1&0\\0&1&0&0\\1&0&0&0\end{pmatrix},\qquad \alpha_y=\begin{pmatrix}0&0&0&-i\\0&0&i&0\\0&-i&0&0\\i&0&0&0\end{pmatrix},$$

$$\alpha_z=\begin{pmatrix}0&0&1&0\\0&0&0&-1\\1&0&0&0\\0&-1&0&0\end{pmatrix},\qquad \beta=\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&-1&0\\0&0&0&-1\end{pmatrix}. \tag{19}$$

Let us assume the solution

$$\psi=\begin{pmatrix}A_1\\A_2\\A_3\\A_4\end{pmatrix}e^{i\mathbf{k}\cdot\mathbf{r}} \tag{20}$$

where the A_λ are functions of the time and $k_x=k_{0x}+\frac{\epsilon Et}{\hbar}$ as before. For convenience, k_z will be taken to be zero to simplify the spinor equations. This does not cause any loss of generality. The substitution of eq (20) into (19) yields

$$\hbar ck_x\begin{pmatrix}A_4\\A_3\\A_2\\A_1\end{pmatrix}+i\hbar ck_y\begin{pmatrix}-A_4\\A_3\\-A_2\\A_1\end{pmatrix}+mc^2\begin{pmatrix}A_1\\A_2\\-A_3\\-A_4\end{pmatrix}=-i\hbar\frac{d}{dt}\begin{pmatrix}A_1\\A_2\\A_3\\A_4\end{pmatrix}. \tag{21}$$

This is equivalent to the relations

$$\begin{aligned}
&-i\frac{dA_1}{dt}+\frac{mc^2}{\hbar}A_1+c(k_x-ik_y)A_4=0,\\
&-i\frac{dA_2}{dt}+\frac{mc^2}{\hbar}A_2+c(k_x+ik_y)A_3=0,\\
&-i\frac{dA_3}{dt}-\frac{mc^2}{\hbar}A_3+c(k_x-ik_y)A_2=0,\\
&-i\frac{dA_4}{dt}-\frac{mc^2}{\hbar}A_4+c(k_x+ik_y)A_1=0.
\end{aligned} \tag{22}$$

It is seen that A_1 and A_4 are coupled and A_2 and A_3 are coupled.

These equations can be made more symmetrical by taking the linear combinations

$$\phi_1 = A_1 + A_4, \qquad \phi_2 = A_2 + A_3, \qquad \phi_4 = A_1 - A_4, \qquad \phi_3 = A_2 - A_3. \tag{23}$$

Then we obtain

$$\begin{aligned}
&-i\frac{d\phi_1}{dt} + ck_x\phi_1 + \left(\frac{mc^2}{\hbar} + ick_y\right)\phi_4 = 0,\\
&-i\frac{d\phi_4}{dt} - ck_x\phi_4 + \left(\frac{mc^2}{\hbar} - ick_y\right)\phi_1 = 0,\\
&-i\frac{d\phi_2}{dt} + ck_x\phi_2 + \left(\frac{mc^2}{\hbar} - ick_y\right)\phi_3 = 0,\\
&-i\frac{d\phi_3}{dt} - ck_x\phi_3 + \left(\frac{mc^2}{\hbar} + ick_y\right)\phi_2 = 0.
\end{aligned} \tag{24}$$

These spinor components have a somewhat similar time-dependence as the Klein-Gordon case. This is illustrated by examining ϕ_1 and ϕ_4. If the dimensionless quantities, eq (11), are used and the substitutions

$$\phi_1 = e^{\frac{iu^2}{2}} f, \qquad \phi_4 = e^{\frac{iu^2}{2}} g \tag{25}$$

are made, then

$$-i\frac{df}{du} + 2uf + \left(\frac{\hbar}{c\epsilon E}\right)^{1/2}\left(\frac{mc^2}{\hbar} + ick_y\right)g = 0, \qquad -i\frac{dg}{du} + \left(\frac{\hbar}{c\epsilon E}\right)^{1/2}\left(\frac{mc^2}{\hbar} - ick_y\right)f = 0. \tag{26}$$

These equations are equivalent to

$$\frac{d^2f}{du^2} + 2i\frac{d}{du}(uf) + a^2 f = 0, \qquad g = -i\left(\frac{\hbar}{c\epsilon E}\right)^{1/2}\left(\frac{mc^2}{\hbar} - ick_y\right)\int f du + g_0. \tag{27}$$

The function f can be represented by a power series,

$$f = \sum_0^\infty b_n u^n. \tag{28}$$

The coefficients of the series are found from the recursion relation

$$\frac{b_{n+2}}{b_n} = -\frac{2i(n+1) + a^2}{(n+1)(n+2)} \tag{29}$$

for both odd and even n. The two constants b_0 and b_1 are determined by the initial values of f and g at zero time. The functions f and g are interchanged in eq (26) and all terms containing i change sign if $e^{-\frac{iu^2}{2}}$ is used (charge conjugation). The components A_1 and A_4 are given by

$$\begin{aligned}
A_1 &= \frac{1}{2}e^{\pm\frac{iu^2}{2}}(f+g),\\
A_4 &= \frac{1}{2}e^{\pm\frac{iu^2}{2}}(f-g).
\end{aligned} \tag{30}$$

The components A_2 and A_3 can be expressed in a similar way. The solution of the time independent Dirac equation for a uniform field has been treated by Sauter [2] who has a detailed description of the solution of equations similar in form to eq (26).

The two arbitrary constants b_0 and b_1 for the Klein-Gordon solution and f_0 and g_0 for the Dirac solution can be specified by normalizing the probability per unit volume and by the relative amounts of positive and negative charge at the initial time. For example, it would be possible to start with a "pure" charge at zero time. The charge could be positive (with no negative charge density) or negative (with no positive charge density). At later time, both charge densities are present, and the charge densities vary with time, but the net charge density is constant,

$$\rho = \rho_+ - \rho_- = \text{constant}.$$

These charge states are discussed by Feshbach [1] and by Foldy [3].

This examination of the time-dependent equations could be extended to the example of combined electric and magnetic fields. There are two Lorentz invariants [4],

$$E^2 - B^2 = I_1,$$

$$\mathbf{E} \cdot \mathbf{B} = I_2. \tag{31}$$

If $\mathbf{E} \cdot \mathbf{B} = 0$, but $I_1 \neq 0$, it is possible to find a Lorentz frame in which there is only an electric or a magnetic field. If $E > B$ (Gaussian units), a frame exists in which there is only an electric field. If $E < B$, a frame exists in which there is only a magnetic field.

4. References

[1] H. Feshbach and F. Villars, Revs. Modern Phys. **30**, 24 (1958).

[2] F. Sauter, Z. Physik **69**, 742 (1931).

[3] Quantum Theory, **III**, 40, Ed. by D. R. Bates (Academic Press, New York, N.Y., 1962).

[4] W. Panofsky and M. Phillips, Classical Electricity and Magnetism, p. 362 (Addison-Wesley Publishing Company, Reading, Mass., 1955).

(Paper 72B1–258)

JOURNAL OF RESEARCH of the National Bureau of Standards—B. Mathematical Sciences
Vol. 72B, No. 1, January–March 1968

Analysis of a Market Split Model*

J. M. McLynn, A. J. Goldman, P. R. Meyers, and R. H. Watkins****

Institute for Basic Standards, National Bureau of Standards, Washington, D.C. 20234

(May 9, 1967)

A mathematical analysis is given for a class of models describing how a "market" (i.e., some subset of the consuming public) might divide its patronage among p competing products ($p > 1$). The analysis is confined to the question of how the respective shares of market change with respect to changes in the variables describing the competing products. The split fractions which define the share of market are assumed to be functions of the choice-influencing attributes of *all* the competing products. The elasticities of the split fractions with respect to these attributes are assumed to be functions only of the split fractions themselves. Some functional forms (including the linear case) leading to self-consistent models are analyzed and their solutions derived.

Key Words: Demand, elasticity, mathematical economics, partial differential equations.

1. Introduction

This paper is concerned with a class of mathematical models of how the "market" (i.e., the consuming public) might divide itself among several competing products

$$P_1, P_2, \ldots, P_p$$

where $p > 1$. Subscripts j, k, m, n, J will be used as "product indices," taking values between 1 and p inclusive.

The notation

$$\mathbf{w} = (w_1, w_2, \ldots, w_p)$$

will be used for the vector of *split fractions*

$$w_j = \text{fraction of market which selects } P_j; \tag{1.1}$$

these necessarily satisfy the conditions

$$w_j \geq 0, \tag{1.2}$$

$$\sum_{j=1}^{p} w_j = 1. \tag{1.3}$$

With the further notation

$$M = \text{total market size}, \tag{1.4}$$

$$M_j = \text{size of } P_j\text{'s market share} \tag{1.5}$$

*Supported by the Office of High-Speed Ground Transportation, Department of Commerce. No official endorsement implied.

**Davidson, Talbird, and McLynn, Bethesda, Md., 4903 Auburn Ave., Bethesda, Maryland 20014.

we then have

$$M_j = w_j M. \tag{1.6}$$

The attributes of P_j which influence the market split are described by a vector

$$\mathbf{x}_j = (x_{1j}, x_{2j}, \ldots, x_{n(j),j})$$

of real parameters. To clarify the role of the first subscript of x_{ij}, we note that x_{11} need not have the same interpretation (e.g., durability) as x_{12}, and might even refer to some quality of P_1 which is meaningless for P_2. The ensemble of *all* the x's (for all products) will be denoted $\mathbf{x}$.

The market share of P_j can depend on the relative attractiveness of the other products, and so we have $w_j(\mathbf{x})$ and $M_j(\mathbf{x})$ rather than $w_j(\mathbf{x}_j)$ and $M_j(\mathbf{x}_j)$. The total market size is not assumed constant, so that in general $M = M(\mathbf{x})$. We make the *smoothness assumption* that the functions $w_j(\mathbf{x})$ and $M(\mathbf{x})$ have first-order partial derivatives, so that the same is true of $M_j(\mathbf{x})$ as well.

This hypothesis is not made explicit merely for the sake of mathematical rigor; it has substantive content. For example, the equality of right-hand and left-hand derivatives can be interpreted as ruling out different degrees of "stickiness" associated with gains and with losses in market share. Also, if P_1 and P_2 are "strictly comparable" in the sense that $\mathbf{x}_1$ and $\mathbf{x}_2$ have the same number of components and corresponding components have identical interpretations, and if P_1 is inferior to P_2 with respect to *each* of these components, the smoothness assumption rules out any automatic conclusion of a zero market share for P_1. A nonzero market share for P_1 might seem at first to represent irrational consumer behavior. However, continuous and nonextreme variation of market shares seems likely to be typical of *real* situations, where different consumers appraise products differently (e.g., may "perceive" different values for the x_{ij}'s), and where all significant choice-influencing factors are unlikely to be fully represented (or even represented at all) in any usable model.

Two apparently innocuous model assumptions will be stated next. They assert that the x_{ij}'s have been redefined (if necessary) so that

$$x_{ij} > 0, \tag{1.7}$$

and so that increasing x_{ij} makes P_j *less* attractive than before (or at least no more attractive), thus tending to decrease w_j and to increase the other w_k's. Formally,

$$\partial w_j / \partial x_{ij} \leq 0, \tag{1.8}$$

$$\partial w_k / \partial x_{ij} \geq 0 \qquad \text{for } k \neq j. \tag{1.9}$$

The only purpose of (1.7) is to permit transformation to new variables

$$y_{ij} = \log x_{ij} \tag{1.10}$$

for subsequent simplifications.

We recall that the *elasticity* of a function $Q(\mathbf{x})$, with respect to changes in x_{ij}, is defined (when $Q \neq 0$) as

$$E_{ij}(Q) = (\partial Q / \partial x_{ij}) / (Q / x_{ij}) = Q^{-1} \partial Q / \partial y_{ij}, \tag{1.11}$$

i.e., as the (limiting) rate of relative change in Q, dQ/Q, per unit relative change in x_{ij}, dx_{ij}/x_{ij}. Q might be associated with one of the products P_k, where either $k = j$ (self-elasticity for P_j) or $k \neq j$ (cross-elasticity) might hold.

It is traditional in economics to consider the elasticities $E_{ij}(M_k)$, and to focus on the M_k's. From (1.6), however, we have

$$E_{ij}(M_k) = E_{ij}(M) + E_{ij}(w_k). \tag{1.12}$$

This suggests—as does (1.6) itself—a decomposition of effort in which one focuses separately on M and on $\mathbf{w}$. Such a suggestion is supported by the fact that variables outside $\mathbf{x}$, e.g., level of institutional advertising by a trade association, or price levels held constant across an industry by regulatory agencies, may affect M in a way largely irrelevant to the competitive aspects represented by $\mathbf{w}$. *In this paper, we focus attention exclusively on* $\mathbf{w}$. It was for this reason that we did not list, together with (1.8), the analogous

$$\partial M/\partial x_{ij} \leq 0.$$

If a satisfactory model dealing with $\mathbf{w}$ is arrived at, then at least same information about $M(\mathbf{x})$ could be inferred from the plausible hypothesis that

$$\partial M_j/\partial x_{ij} \leq \partial M/\partial x_{ij}$$

which by (1.6) can be written (for $w_j \neq 1$)

$$(1-w_j)^{-1}\partial w_j/\partial x_{ij} \leq M^{-1}\partial M/\partial x_{ij} \leq 0. \tag{1.13}$$

Since we are dealing with a model for $\mathbf{w}$, the following *irredundancy hypothesis* becomes innocuous: For each pair (i, j), with $1 \leq j \leq p$ and $1 \leq i \leq n(j)$, there is at least one product P_k for which

$$\partial w_k/\partial x_{ij} \neq 0. \tag{1.14}$$

(Otherwise the parameter x_{ij} has no influence on the market split, and so can and should be omitted from the model.) It follows that such a P_k can be chosen distinct from P_j, for if

$$\partial w_k/\partial x_{ij} = 0$$

for all k with $k \neq j$, then by (1.3)

$$\partial w_j/\partial x_{ij} = \partial(1 - \sum_{k \neq j} w_k)/\partial x_{ij} = 0$$

would hold as well.

The next model assumptions deal with the question of which points in $(w_1, w_2, \ldots, w_p)$-space, among those satisfying (1.2) and (1.3), are *attainable* in the sense of arising as $\mathbf{w}(\mathbf{x})$ for some $\mathbf{x}$. For any product P_j, consider the point defined by

$$w_j = 1;\ w_k = 0 \qquad \text{for } k \neq j. \tag{1.15}$$

The *first* assumption asserts that each of these p points (i.e., for $j = 1, 2, \ldots, p$) is in the attainable region. While we require only that these points be limit points (rather than members) of the attainable region, it is convenient not to have to repeat this distinction everywhere. Therefore, we will speak of points as "in" the region even when only the weaker condition holds. The intended interpretation is that none of the products has a guaranteed minimum market share, nor is any of them artificially precluded from coming arbitrarily close to gaining the entire market if its superiority

would lead to this result. For the *second* assumption (which actually subsumes the first) consider, for any distinct products P_j and P_k and any number w with $0 \leq w \leq 1$, the point defined by

$$w_j = w,\ w_k = 1 - w,\ w_m = 0 \qquad \text{for } m \neq j,\ k. \tag{1.16}$$

The assertion now is that each such point is also a limit point of the attainable region, i.e., any two products can come arbitrarily close to capturing the entire market and sharing it in a prescribed ratio. These two assertions will be called the *competitiveness hypotheses*, since they are most naturally interpreted as referring to (i) the degree of direct competitive confrontation among the products, and (ii) the absence of "constraints on competition" which would limit the variety of market splits possible under changes in the relative merits of the products. The *third* competitiveness hypothesis, which applies only when $p > 2$ and which then subsumes the others, makes the analogous assertion for any *triple* of distinct products.

For verifying that the models and solutions determined later actually *do* satisfy the competitiveness hypothesis, we must be more explicit than the limiting (1.7) about the extent of the attainable region in **x**-space. (This region would of course be altered by rescaling or other admissable transformations of the x's.) Note that such a region need not be a Cartesian product of regions in $\mathbf{x}_j$-space for $j = 1, 2, \ldots, p$, since for example products might compete as customers for one or more scarce resources important to their quality. Even with the parameters for all but a single P_j fixed, the resulting attainable region in $\mathbf{x}_j$-space need not be a Cartesian product; it may have a "curved" boundary representing "tradeoffs" among x_{ij}'s "at the limits" set by available technology and resources. Also, parameters x_{ij} may well have bounds, beyond which one would choose to speak not of P_j but rather of a "different" product perhaps competing in a different market.

There are many assumptions, on the attainable region in **x**-space, which will permit the desired verifications to be carried out. The particular hypothesis chosen for definiteness, though fairly natural mathematically, is perhaps not fully satisfactory in the light of the preceding paragraph. It's somewhat complicated statement is deferred to the point in the analysis (near the end of sec. 3) at which it is invoked.

The final assumption is the one which actually specifies the form of the model. Consider the elasticities $E_{ij}(w_k)$. They are (initially unknown) functions of the $\sum_{j=1}^{p} n(j)$ components of **x**, but it would clearly be much more convenient *if* they could be determined by observing only the p split fractions (the components of **w**). This suggests examining models of the form

$$E_{ij}(w_k) = F_{ijk}(\mathbf{w}),$$

which by (1.11) is equivalent to the system

$$\partial w_k / \partial y_{ij} = w_k F_{ijk}(\mathbf{w}) \tag{1.17}$$

of partial differential equations.

It is natural to begin with the simple case in which each F_{ijk} is *linear*, so that (1.17) becomes

$$\partial w_k / \partial y_{ij} = \sum_{m=1}^{p} b_{ijkm} w_k w_m \tag{1.18}$$

where the b's are constants. This is no less general than the (possibly) *in*homogeneous linear case

$$F_{ijk}(\mathbf{w}) = a_{ijk} + \sum_{m} b'_{ijkm} w_m,$$

since the latter can be brought into the form of (1.18) by setting

$$b_{ijkm} = b'_{ijkm} + a_{ijk}$$

and appealing to (1.3).

We shall deal with a generalization in which the F_{ijk} are *separable*, i.e.,

$$F_{ijk}(\mathbf{w}) = \sum_m b_{ijkm} g_m(w_m),$$

and in fact with the further generalization given by

$$\partial w_k / \partial y_{ij} = \sum_{m=1}^{p} b_{ijkm} f_k(w_k) g_m(w_m) \tag{1.19}$$

where the functions f_k and $g_k (k = 1, 2, \ldots, p)$, defined on $0 \leq w \leq 1$, satisfy

$$f_k(0) = g_k(0) = 0 \tag{1.20}$$

and have continuous derivatives f'_k and g'_k such that

$$f'_k > 0,\ g'_k > 0. \tag{1.21}$$

We call this "the model," and will use this term when referring to eqs (1.19) to (1.21). These last two conditions are of course satisfied for the particular choices

$$f_k(w) = g_k(w) = w$$

which specialize the model eqs (1.19) to (1.18). It will be clear from the proofs to come that finitely many points of exception to (1.21) can be permitted.

Our analysis, of the class of models described by (1.19) and the other assumptions listed above, will be *complete* in the following sense: Those models in the class which are *consistent* (i.e., have at least one solution $\mathbf{w}(\mathbf{x})$) will be identified, and for each of these consistent models the general solution will be given in explicit form. Those parts of the argument common to the cases $p > 2$ and $p = 2$ are presented in section 2, but these cases then require separate treatment; section 3 treats situations with three or more competing products, while section 4 deals with the case of just a pair of competitors.

There are three reasons for passing from the linear model (1.18) to the (possibly) nonlinear (1.19). One is simply intellectual curiosity as to how the generalization might affect the analysis. Second, is the possibility that some special insight into the competitive situation at hand will strongly suggest that linearity is implausible. Third, if it should prove impossible to obtain a satisfactory "fit" to empirical data using the linear model, then perhaps more parameters (which can be adjusted to improve the fit) can be smuggled in *via* the f_k's and g_k's. The conclusions of section 3, however, show that the second and third of these hopes are *in vain* when $p > 2$; the only consistent models are a subclass of the linear ones given by (1.18). For $p = 2$, however, the class of consistent models is shown (in sec. 4) to contain many nonlinear ones.

In the application motivating this work, the "market" in question is to consist of a single "cell" in some stratification of the population of travelers between a particular origin and a particular destination. The "products" are the services offered by the various transport alternatives; the latter might be taken as the traditional transportation "modes" (air, rail, bus, private auto) plus whatever novelties social and technological change may produce, or might reflect a finer classification (e.g., particular auto routes, particular airlines, first-class versus coach service). The components of $\mathbf{x}$ might be measures of trip time, trip cost, variability from published schedules, trip fatigue, frequency and severity of accidents, etc. Validation and subsequent use (for prediction)

289-930 OL-68—4

of such a model would of course require operationally meaningful specifications of the transport alternatives (more generally, the products) and of the x's, and also appropriate "calibration" based on empirical data. In the present paper, however, we are solely concerned with the mathematical consequences of the model's assumptions. In particular, the interpretive discussion of the model is concluded at this point, the remaining sections of the paper consisting of mathematical analysis only.

The reader who works through the following derivations is bound to be struck by the very heavy use of the competitiveness hypotheses, especially in showing the strong interconnectedness of all the products early in section 3. As a topic for further investigation, we would suggest the problem of replacing these hypotheses by fruitful but weaker assumptions on what market splits are theoretically attainable, and of determining the resulting classes of consistent models and their solutions. Those consistent models and associated solutions developed in this paper will remain valid, the technical change being that some of those b's which are not forced to be zero by model hypotheses other than the competitiveness hypothesis, might actually be zero. The essential question, however, is that of what *additional* models might prove consistent under the relaxed hypotheses.

2. Preliminaries

We begin this section by showing that

$$\partial(\partial w_k/\partial y_{ij})/\partial y_{IJ} = \partial(\partial w_k/\partial y_{IJ})/\partial y_{ij}. \tag{2.1}$$

As is well known, to prove this it suffices to show that the two second-order partial derivatives exist and are continuous. For the derivatives on the left in (1.19) to exist, $\mathbf{w}(\mathbf{x})$ must be continuous. Since the f's and g's are continuous, it follows from (1.19) that all of the first-order partial derivatives of $\mathbf{w}(\mathbf{x})$ are continuous. We can evaluate the left-hand side of (2.1) by applying the chain rule to (1.19):

$$\partial(\partial w_k/\partial y_{ij})/\partial y_{IJ} = \sum_m b_{ijkm}\{f_k'(w_k)g_m(w_m)\,\partial w_k/\partial y_{IJ} + f_k(w_k)g_m'(w_m)\,\partial w_m/\partial y_{IJ}\}. \tag{2.2}$$

Since the f's and g's and their derivatives are continuous, and the first-order partial derivatives on the right in (2.2) were just proved continuous, it follows that the left-hand side of (2.1) is continuous; similarly for the right-hand side.

The derivatives on the right in (2.2) can be evaluated using (1.19); the resulting expression for the *left* side of (2.1) is

$$\sum_m \sum_n b_{ijkm}b_{IJkn}f_k'(w_k)g_m(w_m)f_k(w_k)g_n(w_n) + \sum_m \sum_n b_{ijkm}b_{IJmn}f_k(w_k)g_m'(w_m)f_m(w_m)g_n(w_n). \tag{2.3}$$

The corresponding expression for the *right* side of (2.1) can be obtained from (2.3) by interchanging (i, j) and (I, J); the first of its two summands, after interchanging the dummy indices m and n, coincides with the first summand of (2.3). Thus (2.1) yields

$$f_k(w_k)\sum_m \sum_n \{b_{ijkm}b_{IJmn} - b_{IJkm}b_{ijmn}\}\ g_m'(w_m)f_m(w_m)g_n(w_n) = 0. \tag{2.4}$$

We next show that a consistent model is *sparse*, i.e., that most of the b's must vanish. Specifically we show that

$$b_{ijkk} = 0 \tag{2.5}$$

and that

$$b_{ijkm} = 0 \qquad (j \neq k,\ m), \tag{2.6}$$

so that only the b_{ijjk}'s and b_{ijkj}'s with $k \neq j$ can possibly be nonzero. For this purpose, first note from (1.3) that

$$\sum_k \partial w_k/\partial y_{ij} = \partial\left(\sum_k w_k\right)/\partial y_{ij} = 0.$$

Substituting (1.19) into this, we obtain

$$\sum_k \sum_m b_{ijkm} f_k(w_k) g_m(w_m) = 0. \tag{2.7}$$

Because the point defined by $w_k = 1$ and $w_m = 0$ for $m \neq k$ is a limit point of the attainable region, while f_k and g_m are continuous and $g_m(0) = 0$, it follows from (2.7) that

$$b_{ijkk} f_k^{(1)} g_k^{(1)} = 0.$$

Since (1.20) and (1.21) imply $f_k(1) g_k(1) > 0$, (2.5) is proved.

Suppose now that (j, k, m) are distinct. By (1.9), we have

$$\sum_n b_{ijkn} f_k(w_k) g_n(w_n) = \partial w_k/\partial y_{ij} \geq 0. \tag{2.8}$$

For any w with $0 \leq w \leq 1$, the point defined by

$$w_k = w,\ w_m = 1 - w,\ w_n = 0 \text{ for } n \neq k,\ m$$

is a limit point of the attainable region; using this, (2.5), and the continuity of the f's and g's, we see that (2.8) implies

$$b_{ijkm} f_k(w) g_m(1-w) \geq 0$$

for $0 \leq w \leq 1$, which in turn implies

$$b_{ijkm} \geq 0. \tag{2.9}$$

Similarly (2.7) implies

$$b_{ijkm} f_k(w) g_m(1-w) + b_{ijmk} f_m(1-w) g_k(w) = 0. \tag{2.10}$$

But by (2.9) both b's in (2.10) are nonnegative, while by (1.20) and (1.21) the f-values and g-values are strictly positive for $0 < w < 1$; hence (2.6) must hold.

Equations (2.5) and (2.6) have a number of consequences. *First*, we see that for consistent models, (1.19) must have the form

$$\partial w_k/\partial y_{ij} = b_{ijkj} f_k(w_k) g_j(w_j) \qquad (k \neq j), \tag{2.11}$$

$$\partial w_j/\partial y_{ij} = \sum_{m \neq j} b_{ijjm} f_j(w_j) g_m(w_m). \tag{2.12}$$

Since the points defined by $w_j + w_k = 1$ together with (1.2) and (1.3) are limit points of the attainable region, it follows from (2.11) and (1.9) that

$$b_{ijkj} \geq 0. \tag{2.13}$$

Second, it follows that the only interesting case of (2.10) is

$$b_{ijkj}f_k(w)g_j(1-w) + b_{ijjk}f_j(1-w)g_k(w) = 0. \tag{2.14}$$

From this and (2.13) it follows that

$$b_{ijjk} \leqslant 0. \tag{2.15}$$

Another implication of (2.14) is

$$b_{ijkj} = 0 \qquad \text{iff } b_{ijjk} = 0, \tag{2.16}$$

a result useful in studying the pattern of nonzero b's. From (2.11) we can infer that constant nonzero elasticities $E_{ij}(w_k)\,(k \neq j)$ are impossible, while from (2.12) and (2.15) it follows that constant nonzero self-elasticities $E_{ij}(w_j)$ are also impossible. *Third*, we observe that (2.7) becomes

$$\sum_{m \neq j} b_{ijjm}f_j(w_j)g_m(w_m) + \sum_{k \neq j} b_{ijkj}f_k(w_k)g_j(w_j) = 0;$$

a neater form is

$$\sum_{k \neq j} \{b_{ijjk}f_j(w_j)g_k(w_k) + b_{ijkj}f_k(w_k)g_j(w_j)\} = 0. \tag{2.16a}$$

We can also use (2.5) and (2.6) to simplify (2.4). For (j, k, J) distinct, which implies $p > 2$, (2.4) becomes

$$f_k(w_k)\{b_{ijkj}b_{IJjJ}g'_j(w_j)f_j(w_j)g_J(w_J)\} = f_k(w_k)\{b_{IJkJ}b_{ijjJ}g'_J(w_J)f_J(w_J)g_j(w_j)\}. \tag{2.17}$$

This has of course only been proved for the case in which (w_j, w_k, w_J) are the indicated components of some $\mathbf{w}$ which lies in (or . . . by continuity . . . is a limit point of) the attainable region. But by the third competiveness hypothesis, for any nonnegative w_j, w_J with $w_j + w_J < 1$, such a $\mathbf{W}$ is obtained by setting $w_k = 1 - w_j - w_J$; this implies $f_k(w_k) > 0$, so that (2.17) yields (for *distinct* j, k, J)

$$b_{ijkj}b_{IJjJ}g'_j(w_j)f_j(w_j)g_J(w_J) = b_{IJkJ}b_{ijjJ}g'_J(w_J)f_J(w_J)g_j(w_j) \tag{2.18}$$

as valid for any nonnegative (w_j, w_J) with $w_j + w_J < 1$, and hence (by continuity) for $w_j + w_J = 1$ as well.

Next take $j = k \neq J$ in (2.4). Then application of (2.5) and (2.6) yields

$$f_j(w_j)\{g'_J(w_J)f_J(w_J)\Big[\sum_{n \neq J} b_{ijjJ}b_{IJJn}g_n(w_n) - b_{IJjJ}b_{ijjj}g_j(w_j)\Big] + \sum_{m \neq J,\, j} b_{ijjm}b_{IJmJ}g'_m(w_m)f_m(w_m)g_J(w_J)\} = 0,$$

which can be rearranged as

$$f_j(w_j)\{(b_{ijjJ}b_{IJJj} - b_{IJjJ}b_{ijjj})g'_J(w_J)f_J(w_J)g_j(w_j)$$

$$+ \sum_{m \neq J,\, j} [b_{ijjJ}b_{IJJm}g'_J(w_J)f_J(w_J)g_m(w_m) + b_{ijjm}b_{IJmJ}g'_m(w_m)f_m(w_m)g_J(w_J)]\} = 0. \tag{2.19}$$

This has of course only been proved for those cases in which $j \neq J$ and the w's are the components of some $\mathbf{w}$ which lies in or is a limit point of the attainable region.

Now consider any two products P_j and P_J, $j \neq J$. We will call P_j *weakly disconnected* (*strongly disconnected*) from P_J if $\partial w_J/\partial y_{ij} = 0$ holds for some i (for *all* i) with $1 \leq i \leq n(j)$. Clearly strong disconnectedness implies weak disconnectedness. It will now be shown that, conversely, weak disconnectedness implies strong disconnectedness, so that we can speak simply of "disconnectedness" and its opposite, "connectedness." It will also be shown that disconnectedness (and hence connectedness) is a *symmetric* relation, i.e., if P_j is disconnected from P_J, then P_J is disconnected from P_j.

For the proof, assume $\partial w_J/\partial y_{ij} = 0$ for some i. Then $b_{ijJj} = 0$, by (2.11). By the irredundancy hypothesis (used only here!) there is a k, with $k \neq j$, such that $\partial w_k/\partial y_{ij} \neq 0$ and hence by (2.11) such that $b_{ijkj} \neq 0$; thus $k \neq J$. Since (j, k, J) are distinct, we can apply (2.18) to infer that $b_{iJjJ} = 0$ for *all* I with $1 \leq I \leq n(J)$, i.e., that P_J is strongly disconnected from P_j. Applying the same argument with j and J interchanged, we have P_j strongly disconnected from P_J.

3. Analysis for More Than Two Products

We begin the analysis for $p > 2$ by showing that the relation of connectivity, proved symmetric at the end of the previous section, is also *transitive* in the sense that for distinct (j, k, J), if P_j is connected to P_k and P_k is connected to P_J, then P_j is connected to P_J. For the proof, note that for any w with $0 \leq w \leq 1$, the point defined by

$$w_k = w,\ w_J = 1 - w,\ w_m = 0 \text{ for } m \neq k, J$$

is a limit point of the attainable region. From this and (2.19), we have

$$b_{ijjk} b_{iJkJ} g_k'(w) f_k(w) g_J(1-w) + b_{ijjJ} b_{iJJk}\, g_J'(1-w) f_J(1-w) g_k(w) = 0.$$

If P_j were *dis*connected from P_J, the second summand would vanish, leaving

$$b_{ijjk} b_{iJkJ} g_k'(w) f_k(w) g_J(1-w) = 0$$

for $0 \leq w \leq 1$, and thus $b_{ijjk} b_{iJkJ} = 0$. This however is impossible because P_j is connected to P_k, and P_k to P_J (note the use of (2.16)); the proof of transitivity is complete.

Next it will be shown that *total connectivity* holds, i.e., for *any* distinct j and J, P_j and P_J are connected. If not, then since "connectedness" is both symmetric and transitive, the set of p products would decompose into two or more subsets such that

(i) any two products in the same subset are connected, but

(ii) no two products in different subsets are connected. Suppose for example that P_1 and P_2 lie in different subsets S_1 and S_2. Then $\partial w_1/\partial x_{ij} = 0$ unless P_j is in S_1, i.e., w_1 depends only on the parameters of the products in S_1, and similarly for w_2 and S_2. By the first competitiveness hypothesis there exist choices of $\{\mathbf{x}_j : j \in S_1\}$ for which $\mathbf{w}(\mathbf{x})$ has w_1 arbitrarily close to 1, which requires that w_2 be arbitrarily close to 0. This is impossible because the parameters of products in S_1 cannot influence w_2. It follows from this contradiction that, for $p > 2$, total connectivity must hold, i.e., all of the *possibly* nonzero b's (the b_{ijkj}'s and b_{ijjk}'s for $k \neq j$) *are* in fact nonzero. (From this and the argument below (2.16), it follows that for $p > 2$ there can be no *constant* elasticities $E_{ij}(w_k)$ in a consistent model.)

Thus for distinct (j, k, J), the b's in (2.18) are nonzero. For $w_j > 0$ and $w_J > 0$, (2.18) can be written

$$b_{ijkj} b_{iJjJ} g_j'(w_j) f_j(w_j)/g_j(w_j) = b_{iJkJ} b_{ijjJ} g_J'(w_J) f_J(w_J)/g_J(w_J).$$

The left side is a function of w_j only, the right one a function of w_J only. Since $p > 2$, it follows that both are *constant*, and since the b's are nonzero, there exist (necessarily positive) constants d_j such that for $w_j > 0$

$$f_j(w_j)g_j'(w_j)/g_j(w_j) = d_j,$$

i.e. (by continuity for $w_j = 0$ also)

$$f_j = d_j g_j / g_j'. \tag{3.1}$$

Thus the f's are uniquely determined by the g's (in a consistent model).

At this point it is convenient to introduce the normalization

$$g_m(1) = 1 \qquad (m = 1, 2, \ldots, p), \tag{3.2}$$

which is possible since $g_m(1) > 0$, i.e., we can replace b_{ijkm} with $b_{ijkm}g_m(1)$ and g_m with $g_m/g_m(1)$.

Now we return to (2.14), with (j, k) distinct, and apply (3.1) to obtain

$$(b_{ijkj}d_k g_k(w)g_j(1-w)/g_k'(w) + (b_{ijjk}d_j g_j(1-w)g_k(w))/g_j'(1-w) = 0.$$

Thus for $0 < w < 1$, and hence by continuity for $0 \leq w \leq 1$,

$$b_{ijkj}d_k g_j'(1-w) + b_{ijjk}d_j g_k'(w) = 0. \tag{3.3}$$

Indefinite integration with lower limit zero gives

$$b_{ijjk}d_j g_k(w) - b_{ijkj}d_k g_j(1-w) = -b_{ijkj}d_k, \tag{3.4}$$

where (3.2) has been used to evaluate the right-hand side. Setting $w = 1$, we have

$$b_{ijjk}d_j = -b_{ijkj}d_k. \tag{3.5}$$

Substitution of this into (3.4) yields

$$g_k(w) + g_j(1-w) = 1 \qquad (k \neq j). \tag{3.6}$$

Since $p > 2$, this implies the existence of a *single* function $g(w)$ such that

$$g_k(w) = g(w) \qquad \text{for } k = 1, 2, \ldots, p; \tag{3.7}$$

i.e., the g's coincide.

Now consider any distinct (j, k, J). The third competitiveness hypothesis, applied to (2.19), shows that

$$f_j(w)\{(b_{ijjJ}b_{iJjj} - b_{iJjJ}b_{ijjj})g_J'f_J g_j(w)$$

$$+ b_{ijjJ}b_{iJJk}g_j'(w_J)f_J(w_J)g_k(w_k) + b_{ijjk}b_{iJkJ}g_k'(w_k)f_k(w_k)g_J(w_J)\} = 0$$

holds if $w_j + w_k + w_J = 1$. But by (3.1) $g_j'f_J = d_J g_J$, so the last equation can be written as

$$f_j(w_j)g_J(w_J)\{(b_{ijjJ}b_{iJjj} - b_{iJjJ})b_{ijjj}d_J g_j(w_j) + b_{ijjJ}b_{iJJk}d_J g_k(w_k) + b_{ijjk}b_{iJkJ}d_k g_k(w_k)\} = 0.$$

Thus if $w_j + w_k + w_J = 1$, then

$$(b_{jjJ}b_{JJJ} - b_{JJJ}b_{jjJ})d_J g_j(w_j) + b_{jjJ}b_{JJJk}d_J g_k(w_k) + b_{jjk}b_{JJkJ}d_k g_k(w_k) = 0$$

holds if $w_j > 0$ and $w_J > 0$, and hence (by continuity) even without this extra hypothesis. Taking $w_k = 1$ leads to

$$b_{jjJ}b_{JJJk}d_J + b_{jjk}b_{JJkJ}d_k = 0.$$

But by (3.5),

$$b_{JJkJ}d_k = -b_{JJJk}d_J,$$

so the preceding equation becomes

$$b_{JJJk}d_J(b_{jjJ} - b_{jjk}) = 0 \qquad (j, k, J \text{ distinct}).$$

Since $d_J \neq 0$, this implies the existence of constants b_{ij} (necessarily negative, by (2.15) and total connectivity) such that

$$b_{jjk} = b_{ij} \qquad \text{for all } k \neq j. \tag{3.8}$$

We turn now to (2.16a). By (3.1), it becomes

$$g_j(w_j) \sum_{k \neq j} g_k(w_k)\{b_{jjk}d_j/g_j'(w_j) + b_{jkj}d_k/g_k'(w_k)\} = 0,$$

which by (3.5) can be written

$$g_j(w_j)d_j \sum_{k \neq j} b_{jjk}g_k(w_k)\{1/g_j'(w_j) - 1/g_k'(w_k)\} = 0,$$

and then by (3.8) can be written

$$g_j(w_j)d_j b_{ij} \sum_{k \neq j} g_k(w_k)\{1/g_j'(w_j) - 1/g_k'(w_k)\} = 0. \tag{3.9}$$

Choose any distinct (j, k, J). Then the third competitiveness hypothesis, applied to (3.9) shows that for $w_j + w_k + w_J = 1$,

$$g_k(w_k)\{1/g_j'(w_j) - 1/g_k'(w_k)\} + g_J(w_J)\{1/g_j'(w_j) - 1/g_j'(w_J)\} = 0$$

if $w_j > 0$, and hence (by continuity) also if $w_j = 0$. Choosing

$$w_k = w,\ w_J = 1 - w,\ w_j = 0,$$

and applying (3.7), we have

$$g(w)\{1/g'(0) - 1/g'(w)\} + g(1-w)\{1/g'(0) - 1/g'(1-w)\} = 0,$$

which by (3.6) and the result of differentiating it becomes

$$\{g(w) + g(1-w)\}\{1/g'(0) - 1/g'(w)\} = 1/g'(0) - 1/g'(w) = 0.$$

This implies $g'(w) = g'(0)$ for $w > 0$, i.e., g' is *constant*. Thus g is *linear*, and since $g(0) = 0$ and $g(1) = 1$ we have

$$g(w) = w. \tag{3.10}$$

By (3.1),

$$f_j(w) = d_j w. \tag{3.11}$$

Thus every consistent model is a *linear* one in the sense of (1.17)! By (2.11), (3.5), (3.8), and (3.10–11) we have

$$\partial w_k/\partial y_{ij} = b_{ijkj} d_k w_k w_j$$

$$= -b_{ijjk} d_j w_k w_j = -b_{ij} d_j w_k w_j$$

for $k \neq j$, while use of (2.12) leads to

$$\partial w_j/\partial y_{ij} = \sum_{m \neq j} b_{ijjm} d_j w_j w_m$$

$$= b_{ij} d_j w_j \sum_{m \neq j} w_m = b_{ij} d_j w_j (1 - w_j).$$

Both forms can be combined, with the aid of the Kronecker delta, in

$$\partial w_k/\partial y_{ij} = b_{ij} d_j w_k (\delta_{jk} - w_j). \tag{3.12}$$

We now proceed to the explicit solution of (3.12). We have

$$(1/w_k)\, dw_k = (1/w_k) \sum_{i,j} (\partial w_k/\partial y_{ij})(dy_{ij}).$$

$$= \sum_{i,j} b_{ij} d_j (\delta_{jk} - w_j)(dy_{ij}).$$

Therefore

$$dw_k/w_k - dw_1/w_1 = \sum_{i,j} b_{ij} d_j (\delta_{jk} - \delta_{j1})(dy_{ij}).$$

$$= \sum_i b_{ik} d_k (dy_{ik}) - \sum_i b_{i1} d_1 (dy_{i1}).$$

There is therefore a constant c_k such that

$$\log (w_k/w_1) = \sum_i b_{ik} d_k y_{ik} - \sum_i b_{i1} d_1 y_{i1} + c_k,$$

and hence such that

$$w_k = C_k w_1 W_k / W_1 \tag{3.13}$$

where

$$C_k = \exp\,(c_k) > 0 \qquad (C_1 = 1),$$

$$W_k = \exp\left(\sum_i b_{ik} d_k y_{ik}\right).$$

From the definition (1.10) of y_{ik}, we have

$$W_k = \left(\prod_i x_{ik}^{b_{ik}}\right)^{d_k}. \tag{3.14}$$

By summing (3.13) over $1 \leq k \leq p$ and applying (1.3), we obtain

$$1 = (w_1/W_1) \sum_k C_k W_k,$$

$$w_k = C_k W_k \Big/ \sum_j C_j W_j. \tag{3.15}$$

We have shown that *if* the model (1.19) is to be consistent for $p > 2$, *then* it has the special form (3.12), and its solutions $\mathbf{w}(\mathbf{x})$ have the form

$$w_k = C_k \left(\prod_i x_{ik}^{b_{ik}}\right)^{d_k} \Big/ \sum_n C_n \left(\prod_i x_{in}^{b_{in}}\right)^{d_n} \tag{3.16}$$

involving parameters

$$d_k > 0,\ b_{ik} < 0,\ C_k > 0 \tag{3.17}$$

where the C's are determined only up to a common positive multiplicative factor. Although (3.12) admits the singular solution $w_k(\mathbf{x}) \equiv 0$ corresponding to $C_k = 0$, this is ruled out by the competitiveness hypothesis.

Conversely, consider *any* sets of b's, C's and d's satisfying (3.17), and *define* $\mathbf{w}(\mathbf{x})$ by (3.16). It is readily verified that (1.2) and (1.3), as well as (3.12), are satisfied. The irredundancy hypothesis is also clearly satisfied. So it only remains to check the third competitiveness hypothesis, which subsumes the others. Consider, then, any distinct (j, k, J) and any nonnegative $(w_j^\circ, w_k^\circ, w_J^\circ)$ summing to 1.

To show (as desired) that the point defined by

$$w_j = w_j^\circ,\ w_k = w_k^\circ,\ w_J = w_J^\circ,\ w_m = 0 \qquad \text{for } m \neq j, k, J \tag{3.18}$$

lies in or at least is a limit point of the attainable region in $\mathbf{w}$-space, it is necessary to be more explicit than the delimiting (1.7) about the extent of the feasible region in $\mathbf{x}$-space. To be definite, we will adopt the following somewhat complicated hypothesis: For each distinct (j, k, J), there exists a triple of parameters $(x_{i(1)j},\ x_{i(2),k},\ x_{i(3),J})$ with

$$1 \leq i(1) \leq n(j),\ 1 \leq i(2) \leq n(k),\ 1 \leq i(3) \leq n(J)$$

. . . we immediately renumber them x_{1j}, x_{1k}, x_{1J} . . . such that for certain fixed settings $x_{im} = x_{im}^\circ > 0$ of all *other* parameters

$$\{x_{im}:\ m \neq j, k, J \quad \text{or} \quad i > 1\},$$

there exist constants

$$x_{1j}^{+} > 0,\ x_{1k}^{+} > 0,\ x_{1J}^{+} > 0$$

with the property that *any* numerical triple (x_{1j}, x_{1k}, x_{1J}) obeying

$$0 < x_{1j} < x_{1j}^{+},\ 0 < x_{1k} < x_{1k}^{+},\ 0 < x_{1J} < x_{1J}^{+} \tag{3.19}$$

forms, together with the fixed settings $x_{im} = x_{im}^{\circ}$, a point $\mathbf{x}^{\circ}$ in the attainable region in $\mathbf{x}$-space.

The proof will involve a limiting process in which

$$x_{1j} \to 0+,\ x_{1k} \to 0+,\ x_{1J} \to 0+ \tag{3.20}$$

while all other x_{im} are maintained at the fixed settings x_{im}°. From this and (3.16–17), we have

$$w_m(\mathbf{x}) \to 0 \qquad \text{for } m \neq j,\ k,\ J,$$

as desired. In view of the fixed settings, we have from (3.16) that

$$w_j = C_j^{*}(x_{1j})^{b_{1j}d_j} / (C_j^{*}(x_{1j})^{b_{1j}d_j} + C_k^{*}(x_{1k})^{b_{1k}d_k} + C_J^{*}(x_{1J})^{b_{1J}d_J} + C^{*}),$$

$$w_k = C_k^{*}(x_{1k})^{b_{1k}d_k} / (C_j^{*}(x_{1j})^{b_{1j}d_j} + C_k^{*}(x_{1k})^{b_{1k}d_k} + C_J^{*}(x_{1J})^{b_{1J}d_J} + C^{*}),$$

$$w_J = C_J^{*}(x_{1J})^{b_{1J}d_J} / (C_j^{*}(x_{1j})^{b_{1j}d_j} + C_k^{*}(x_{1k})^{b_{1k}d_k} + C_J^{*}(x_{1J})^{b_{1J}d_J} + C^{*}),$$

where C_j^{*}, C_k^{*}, C_J^{*} are positive constants and C^{*} a nonnegative constant (zero only when $p = 3$).

One of $(w_j^{\circ}, w_k^{\circ}, w_J^{\circ})$, say the last, must be strictly positive. The limiting process can be chosen so that (3.19) holds, while x_{1j} and x_{1k} are defined in terms of x_{1J} in such a way that

$$w_j(\mathbf{x}) / w_J(\mathbf{x}) = C_j^{*}(x_{1j})^{b_{1j}d_j} / C_J^{*}(x_{1J})^{b_{1J}d_J} = w_j^{\circ} / w_J^{\circ},$$

$$w_k(\mathbf{x}) / w_J(\mathbf{x}) = C_k^{*}(x_{1k})^{b_{1k}d_k} / C_J^{*}(x_{1J})^{b_{1J}d_J} = w_k^{\circ} / w_J^{\circ}.$$

Since all points $\mathbf{w}(\mathbf{x})$ associated with the process lie in the closed bounded set defined by

$$\mathbf{w} \geqslant \mathbf{0},\ \sum_m w_m = w_j + w_k + w_J = 1,$$

these points will have a limit point w^{*} obeying the same conditions, and such that

$$w_j^{*} / w_J^{*} = w_j^{\circ} / w_J^{\circ},\ w_k^{*} / w_J^{*} = w_k^{\circ} / w_J^{\circ}.$$

Thus

$$w_j^{*} = w_j^{\circ},\ w_k^{*} = w_k^{\circ},\ w_J^{*} = w_J^{\circ},$$

i.e., w^{*}, defined as a limit point of the attainable region in $\mathbf{w}$-space, coincides with the point (3.18).

We have thus shown that for $p > 2$, (3.12), (3.16), and (3.17) give precisely the class of consistent models and their solutions.

4. The Two-Product Case

In this section we assume $p=2$. The situation will be shown to be quite different from that with $p>2$, in that there is an abundance of consistent nonlinear models.

It is convenient to introduce the continuous functions

$$h_1(w)=f_1(w)g_2(1-w), \tag{4.1}$$

$$h_2(w)=f_2(w)g_1(1-w), \tag{4.2}$$

so that for $j=1, 2$

$$h_j(0)=h_j(1)=0,\ h_j(w)>0 \text{ for } 0<w<1. \tag{4.3}$$

By (2.11) and (2.12), the model takes the form

$$\partial w_1/\partial y_{i1}=b_{i112}h_1(w_1), \tag{4.4}$$

$$\partial w_1/\partial y_{i2}=b_{i212}h_1(w_1), \tag{4.5}$$

$$\partial w_2/\partial y_{i1}=b_{i121}h_2(w_2), \tag{4.6}$$

$$\partial w_2/\partial y_{i2}=b_{i221}h_2(w_2), \tag{4.7}$$

while (2.14) yields

$$b_{i212}h_1(w)+b_{i221}h_2(1-w)=0, \tag{4.8}$$

$$b_{i121}h_2(w)+b_{i112}h_1(1-w)=0. \tag{4.9}$$

The same argument used (in the second paragraph of section 3) to prove total connectivity when $p>2$, can be readily adapted to show that P_1 and P_2 must be connected. Thus (here (2.16) is used) all the b's in (4.4) through (4.7) are nonzero. From (4.8) and (4.9) we have, for $0<w<1$,

$$b_{i112}/b_{i121}=-h_2(w)/h_1(1-w)=b_{i212}/b_{i221}.$$

Thus there is a constant

$$R<0 \tag{4.10}$$

such that

$$Rh_1(1-w)+h_2(w)=0, \tag{4.11}$$

$$b_{i112}=Rb_{i121},\ b_{i212}=Rb_{i221}. \tag{4.12}$$

The sign of R follows from (4.12) together with (2.13) and (2.15). The simplifying substitutions

$$z_{ij}=b_{ij21}y_{ij} \tag{4.13}$$

then convert the model into

$$\partial w_1/\partial z_{i1}=\partial w_1/\partial z_{i2}=Rh_1(w_1), \tag{4.14}$$

$$\partial w_2/\partial z_{i1}=\partial w_2/\partial z_{i2}=h_2(w_2). \tag{4.15}$$

Furthermore, the positive factor $(-R)$ can be absorbed into h_1, i.e., we can assume $R=-1$ so that (4.14) becomes

$$\partial w_1/\partial z_{i1} = \partial w_1/\partial z_{i2} = -h_1(w_1) \tag{4.16}$$

and (4.11) simplifies to

$$h_2(w) = h_1(1-w). \tag{4.17}$$

Substitution of (4.15) or (4.16) into the differential identity

$$dw_j = \sum_1^{n(1)} (\partial w_j/\partial z_{i1})(dz_{i1}) + \sum_1^{n(2)} (\partial w_j/\partial z_{i2})(dz_{i2})$$

yields

$$(dw_j)/h_j(w_j) = (-1)^j \left[\sum_1^{n(1)} (dz_{i1}) + \sum_1^{n(2)} (dz_{i2})\right]. \tag{4.18}$$

For $j=1, 2$, choose points w_{0j} with

$$0 < w_{0j} < 1,\ w_{01} + w_{02} = 1. \tag{4.19}$$

For $0 < w < 1$, let

$$H_j(w) = \int_{w_{0j}}^{w} (1/h_j(w))dw. \tag{4.20}$$

Then in terms of

$$u = \sum_1^{n(1)} z_{i1} + \sum_1^{n(2)} z_{i2}, \tag{4.21}$$

(4.18) yields

$$H_j(w_j) = (-1)^j(u + c_j) \tag{4.22}$$

where c_j is a constant of integration. However, (4.17) and (4.19) lead to

$$H_2(w) = -H_1(1-w), \tag{4.23}$$

which together with (4.22) and (1.3) yields $c_1 = c_2$. Thus

$$H_j(w_j) = (-1)^j(u + c) \tag{4.24}$$

where c is an arbitrary constant.

It follows from (4.3) that the differentiable functions H_j are strictly increasing, with

$$H_j(0) = -\infty,\ H_j(1) = \infty.$$

They therefore possess differentiable strictly increasing *inverse* functions, denoted $\overline{H}_j$, with

$$\overline{H}_j(-\infty) = 0,\ \overline{H}_j(\infty) = 1.$$

It follows from (4.23) that these functions satisfy the identity

$$\overline{H}_1(-v)+\overline{H}_2(v)=1. \tag{4.25}$$

Finally, from (4.24) we see that the general solution is

$$w_1=\overline{H}_1(-(u+c)), \tag{4.26}$$

$$w_2=\overline{H}_2(u+c), \tag{4.27}$$

where u is defined by (4.21) and c is an arbitrary constant.

To relate this to the general solution (3.16) for $p>2$, we set

$$C=\exp\,(c)>0,$$

follow (3.8) in defining

$$b_{i112}=b_{i1},\ b_{i221}=b_{i2}, \tag{4.28}$$

and introduce the functions

$$K_j(v)=\overline{H}_j\,(\log v). \tag{4.29}$$

Then by (4.12),

$$b_{i121}=b_{i1}/R=-b_{i1},$$

and by (4.13) and (1.10) we have

$$u+c=\log\left[C\prod_1^{n(2)}(x_{i2})^{b_{i2}}\Big/\prod_1^{n(1)}(x_{i1})^{b_{i1}}\right].$$

Thus (4.26) and (4.27) take the form

$$w_1=K_1\left(C^{-1}\prod_1^{n(1)}(x_{i1})^{b_{i1}}\Big/\prod_1^{n(2)}(x_{i2})^{b_{i2}}\right), \tag{4.30}$$

$$w_2=K_2\left(C\prod_1^{n(2)}(x_{i2})^{b_{i2}}\Big/\prod_1^{n(1)}(x_{i1})^{b_{i1}}\right), \tag{4.31}$$

involving the same products as in (3.16). Note that the competitiveness hypothesis has been used to rule out the singular solutions $w_j=0$ and $w_j=1$ of (4.15) and (4.16).

Conversely, assume h_1 and h_2 are continuous functions satisfying (4.3) and (4.17). Using some w_{01} and w_{02} as in (4.19), and any constant c, *define* functions w_1 and w_2 by (4.21), (4.26), and (4.27). They satisfy (1.2), and by (4.25) they also obey (1.3). They are readily shown to be solutions of (4.15) and (4.16). Next set $R=-1$, and for any set of

$$b_{i121}>0,\ b_{i221}<0, \tag{4.32}$$

define the remaining b's by (4.12), define the y's from the z's by (4.13), and the x's from the y's by (1.10). Then w_1 and w_2 satisfy (4.4) through (4.7), and satisfy the irredundancy hypothesis because the b's are nonzero. It remains to show that they obey the competitiveness hypothesis.

Consider any nonnegative pair (w_1^0, w_2^0) summing to 1. It must be shown that $\mathbf{w}^0 = (w_1^0, w_2^0)$ is in or at least a limit point of the attainable region in **w**-space. The situation regarding the attainable region in **x**-space is like that discussed for $p > 2$ near the end of section 3, and we adopt for definiteness the hypothesis about that region analogous to the one chosen earlier for $p > 2$: There are variables $x_{i(1)1}$ and $x_{i(2)2}$, which we immediately make x_{11} and x_{12} by renumbering, and numerical settings $x_{i1} = x_{i1}^0 > 0$ and $x_{i2} = x_{i2}^0 > 0$ for all the *other* x's, and numbers $x_{11}^+ > 0$ and $x_{12}^+ > 0$, such that *any* numerical pair (x_{11}, x_{12}) satisfying

$$0 < x_{11} < x_{11}^+, \; 0 < x_{12} < x_{12}^+$$

forms, together with the fixed settings x_{i1}^0 and x_{i2}^0, a point **x** in the attainable region.

Let the fixed settings z_{i1}^0 and z_{i2}^0 correspond via (1.10) and (4.13) to the x_{i1}^0 and x_{i2}^0. Taking into account the signs in (4.32), we find that there exist intervals

$$(-\infty, z_{11}^+) \text{ and } (z_{12}^+, \infty)$$

such that any z_{11} and z_{12} lying respectively in these intervals form, together with the fixed settings, a point in the attainable region in **z**-space. If now $0 < w_2^0 < 1$, then we can choose such z_{11} and z_{12} so that

$$z_{11} + \sum_2^{n(1)} z_{i1}^0 + z_{12} + \sum_2^{n(2)} z_{i2}^0 + c = H_2(w_2^0),$$

and so $w_2 = w_2^0$ and hence $w_1 = w_1^0$. If $w_2^0 = 0$ we use a limiting process with z_{12} fixed and $z_{11} \to (-\infty)$, while if $w_2^0 = 1$ we use a limiting process with z_{11} fixed and $z_{12} \to \infty$.

This completes the proof that all consistent models and their general solutions have been found. We note (omitting details) that for the linear case

$$f_j(w) = d_j w, \;\; g_j(w) = w,$$

the solution derived above has exactly the same form as that obtained in section 3 for $p > 2$.

(Paper 72B1–259)

JOURNAL OF RESEARCH of the National Bureau of Standards—B. Mathematical Sciences
Vol. 72B, No. 1, January–February 1968

Citation Searching and Bibliographic Coupling With Remote On-Line Computer Access*

Franz L. Alt and Russell A. Kirsch**

Institute for Basic Standards, National Bureau of Standards, Washington, D.C. 20234

(January 30, 1968)

Experiments were performed on a remote, multiple access computer to retrieve bibliographic items based on citation data. The citations were from some 25,000 physics papers. Estimates were made of the relevance of bibliographies derived from such citations. Some extrapolations are made to future systems with remote multiple access capability.

Key Words: Bibliographies, citations, computer, information retrieval, remote consoles, timesharing.

1. Introduction

The use of citation indexing for information retrieval is increasingly arousing the interest of the scientific community. It therefore seems appropriate to document some of the experience which the authors have gained with this tool.

A main purpose of the experiments reported here was to determine whether a citation index can be used effectively by remote access to a computer-stored file, and how this process compares with conventional use in a library. A computer-stored citation index has some obvious advantages; it seemed important to find out whether it involved any unforeseen difficulties or, for that matter, any unexpected benefits.

We shall first discuss citation indexes in general, their characteristics and the use that is made of them. This will enable us to appreciate the built-in advantages of a mechanized index. We shall then describe a number of experiments which we have conducted, and finally enumerate a few conclusions which can be drawn from them. These experiments had the special feature of using the computer remotely; it is this characteristic which distinguishes them from earlier trials of mechanized citation indexing [1, 2].[1]

Remote access to computers [3] is made attractive by two kinds of considerations, which in the literature are not always clearly distinguished, although they differ widely in their effects on the design and economics of the computer system. In one class of cases, long-distance access to a computer is desirable because the computer stores a unique information file (or program). The alternative of storing a copy of the file in a locally used computer may be impractical because of frequent need for updating or revision, or may be uneconomical because the file is so large and/or so infrequently used that the cost of computer storage exceeds the cost of long-distance communication. In another class of cases, the desire for man-machine interaction is the controlling consideration. To match the speed of humans and machine calls for time-sharing, usually among several dozen users (even though the machine does the lion's share of the work). It is normally not practical to assemble so many users in the machine room; but in contrast to the former use,

*Work on this project was supported by the National Science Foundation grant number GN-320.

**American Institute of Physics, 335 E. 45th Street, New York, N.Y. 10017.

[1] Figures in brackets indicate the literature references at the end of this paper.

it is often possible and desirable to share the computer's time only among users in the same city, or even in the same installation, thus almost eliminating the costs of communication. In our work with citation indexing, both considerations—access to a unique file and desirability of man-machine interaction—are present.

2. Characteristics and Use of a Citation Index

A citation index ([4], and refs. cited there) is a list of documents (e.g., scientific papers) which cite (make reference to) other documents. Its main purpose is to find citations to a given paper. The index must contain at least an identification of each citing paper and similar identifications for all cited papers associated with each citing paper. The identification should be unique and unambiguous, or nearly so. There may be additional information if desired; though if there is too much of it, the file will be less economical in serving its primary purpose. The order in which the list is arranged, and the format of its items, also have a decisive effect on the economics of the operation. We shall have more to say about this later.

Figures 1 and 2 show typical entries from two citation indexes. The former is taken from the file of the Technical Information Project (TIP) at Massachusetts Institute of Technology (MIT). The first line is the identification of a *citing* paper: in it, J001 is a symbol arbitrarily assigned to one journal (in this case, Physical Review), the remainder of the line gives the volume and (starting) page number. This identification is obviously unique, and it is unambiguous except in the rare case where two papers start on the same page. Similarly, the block of symbols at the end of the entry gives the identifications of the 38 *cited* papers. (Journals are assigned serial numbers lying between 1 and 999; references to papers not in one of these journals are omitted.) Additional information given in the index consists of title of the citing paper, author(s) and his (their) affiliation(s). There is no additional information for the cited papers. Figure 2 is from the Science Citation Index (SCI) of the Institute for Scientific Information. The identification for both citing and cited

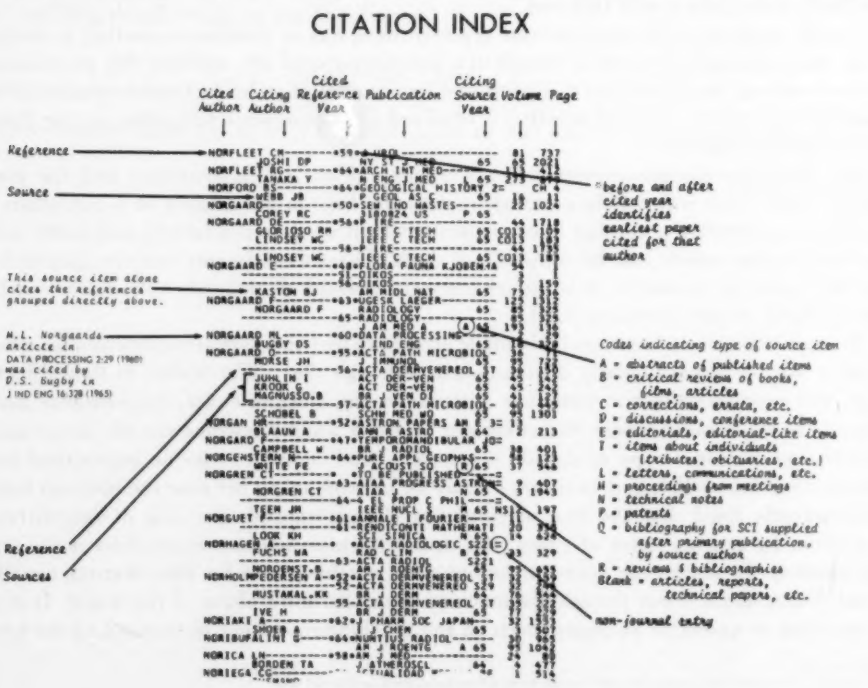

CITATION INDEX
Cited Author
Citing Author
Cited Reference Year
Publication
Citing Source Year
Volume
Page
Reference
Source
"before and after cited year identifies earliest paper cited for that author
This source item alone cites the references grouped directly above.
M.L. Norgaards article in DATA PROCESSING 2:29 (1960) was cited by D.S. Bugby in J IND ENG 16:328 (1965)
Codes indicating type of source item
A = abstracts of published items
B = critical reviews of books, films, articles
C = corrections, errata, etc.
D = discussions, conference items
E = editorials, editorial-like items
I = items about individuals (tributes, obituaries, etc.)
L = letters, communications, etc.
M = proceedings from meetings
N = technical notes
P = patents
Q = bibliography for SCI supplied after primary publication, by source author
R = reviews & bibliographies
Blank = articles, reports, technical papers, etc.
non-journal entry
Reference
Sources

FIGURE 1. *An item from the TIP index.*

PHYSICAL REVIEW
VOLUME 150
J001 V150 P0429
RELATIONSHIP BETWEEN THE AUGMANTED-PLANE-WAVE AND
KORRINGA-KOHN-ROSTOKER METHODS OF BAND THEORY
JOHNSON KEITH H.

J001 V051 P0846	J001 V092 P0603	J001 V092 P1126
J001 V094 P1111	J001 V105 P0108	J001 V124 P1786
J001 V124 P1797	J001 V125 P0109	J001 V128 P0082
J001 V131 P2529	J001 V139 P0760	J001 V145 P0599
J002 V000 P0000	J002 V000 P0000	J002 V000 P0000
J002 V000 P0000	J002 V000 P0000	J003 V086 P0337
J003 V086 P0825	J019 V042 P0276	J021 V013 P0392
J027 V000 P0000	J027 V000 P0000	J027 V000 P0000
J027 V000 P0000	J027 V000 P0000	J384 V064 P0513
J384 V066 P0545	J384 V072 P0345	

FIGURE 2. *A segment of the ISI citation index.*

papers consists of abbreviated journal title, volume and page number; the first author's name and the year of publication are given as additional information for both citing and cited papers. The TIP file is stored in randomly accessible computer memory, from which figure 1 is printed out; the SCI is derived from a file on magnetic tape but is accessible to outsiders mainly in printed form. TIP is arranged by journal, volume and starting page of *citing* papers; SCI is arranged by year of citing paper,[2] and within each year alphabetically by name of first author of *cited* paper.

In TIP, each citing paper is followed by its cited papers. SCI, on the other hand, lists each cited paper, followed immediately by pertinent citing papers. (The Institute for Scientific Information also maintains files in several other arrangements.) It could be argued that the term "citation index" ought to be reserved for the latter form, because unlike any other index, it responds immediately to the basic query "find citations to a given paper." We shall, however, use the term more broadly as applying to any list (such as the TIP index) from which this basic query can be answered without unreasonable effort.

Let us examine the last point more closely. Any request for information from a file may be considered as consisting of at least two parts, of which one specifies the "search-range," i.e., the portion of the file which is to be searched, while the other gives criteria for deciding, for each item in the searched portion of the file, whether the item is or is not wanted as part of the answer to the request. In manual searching these two parts are implicit in the actions of the searcher, where he looks and what he looks for. In the TIP file, where searching is done by computer, they are formalized as two computer statements ("macro-instructions"); one begins with the word **SEARCH,** followed by a list of journal volumes to be searched; the other begins with **FIND** and specifies, e.g., some cited papers; other types of "find" specifications are possible and often useful, such as author's name, words in title, etc. The two parts of the request look as if they played entirely different roles, but logically speaking their functions are quite symmetric. Let A be the set of all papers in the search range, B the set of all those papers in the file which satisfy the "find" specifications; to satisfy the request we have to form the intersection of the sets A and B. The request "search B, find A" would have the same result as "search A, find B." For instance, a request to the TIP index might specify "search Phys. Rev. vol. 135, find citations to Phys. Rev. v. 126 p. 146," the latter being a paper by J. P. Auffray on the magnetic susceptibility of the hydrogen molecule. The result would include the item shown in figure 1, since this paper is in Phys. Rev. (J001) vol. 135, and includes among its citations the one to J001 V 126 P 146. The same request could be made to SCI in the form

[2] To the extent that the file is cumulated and printed annually. This annual cumulation coincides partly but imperfectly with an arrangement on citing year.

289-930 OL-68—5

"search citations to Auffray (Phys. Rev. Vol. 126, p. 146), find citing papers in Phys. Rev. vol. 135." Which of the two forms (or of other possible forms) is chosen will depend on the organization of the file. In TIP all *citing* papers from one journal volume are stored contiguously; therefore the search requests are composed of specific journal volumes. In SCI all *cited* papers of one author are listed in sequence. The latter arrangement is more economical when, e.g., searching for all citations to one given paper, regardless of time; the former is advantageous in requesting, e.g., all papers in the most recent literature citing one of a list of papers, or in limiting the search to journals from certain countries, or journals specializing in certain fields.

3. Types of Requests

In order to appreciate the requirements to be met by a citation index, one should first visualize the modes of consulting it and the reasons for them. For our purposes, the main distinctions will be whether the index is consulted only once for each question or periodically for the same questions; whether questions are asked singly, in batches, or in sequence; what is the time period within which the desired citations should have appeared; and what are the boundaries of the field of knowledge spanned by the citations.

One frequent reason for consulting a citation index will be a scientist's need to obtain the most recent answer to a specific question, when this answer is being revised from time to time. For instance, he may wish to get the latest value for the atomic weight of some element. He knows that this was measured some years ago, and he suspects that it may have been revised since. He enters the index with the latest publication on this subject known to him—perhaps 5 or 10 years old—in the hope that the publication of a subsequent revision would reference the previous result. In such a case the question is asked only once and is a single question (though it may be combined into a batch with other similar questions); the field of knowledge is quite narrow; the time interval of interest extends from the previous paper to the present, with emphasis on the most recent literature. If the scientist continues to work on the same element, he may consult the index periodically with the same question, in which case the time interval of interest runs only from the previous consultation to the present. An organization devoted to up-to-date knowledge of such information, say a data center, may have batches of similar questions, asked periodically, and covering a broad field of knowledge.

A very different problem is that of compiling a bibliography of a subject. Here the researcher may start with a few publications known to him, look up the references cited in them, use this composite list of references to enter the citation index and obtain a longer list of citing papers (which includes his original list), and iterate this procedure several times. At each step it will be desirable to comb out those papers not sufficiently germane to the field. In this application, there is a sequence of consultations of the citation index, each dependent on the results of the previous one and on the inspection of these results by the searcher. The time interval of interest extends over the entire period spanned by the index. There is no special premium on the most recent literature, but it is essential that the period covered be long enough; at least, say, five years, preferably longer. The field of knowledge covered by the index must be at least a little broader than that which is to be spanned by the bibliography, and it is important that this field be covered as completely as possible, including relatively obscure sources.

These two examples will suffice for our argument. There are other important applications of citation indexes—current awareness programs, patent searches, finding reviews of, or corrections to, a given paper, bibliographic coupling, etc. They merely confirm the conclusion that a citation index, to satisfy all major classes of users, must have the following properties: (a) It must cover a continuous time period of at least five years for citing papers. (b) It must be reasonably up-to-date. (c) It must cover its intended field of knowledge as completely as possible, including obscure sources in the field itself and sources in tangential fields which are apt to cite, or be cited in, papers in the principal field itself.

Point (b) requires that there be frequent additions to the index. It is likely that point (c) will require the same thing since it may be difficult to achieve the needed coverage except in successive approximations. Points (a) and (c) imply that the index has to be of large volume; a small incomplete or short-range index has disproportionately small usefulness. The size of the index makes the process of incorporating frequent additions more difficult.

The reason for desiring a coverage of five years is that experience has shown that most citations to a given paper come within five years of its appearance; thereafter the frequency of citation falls off. Thus, with a coverage of less than five contiguous years we are likely to lose some valid retrieval clues.

While neither the SCI nor the TIP index satisfy these requirements completely, both are close enough to make extrapolation of our results to a hypothetical index with completely adequate coverage permissible. The TIP index begins in 1963 for most of its journals and is thus approaching the five-year condition. Indeed, some older volumes are on magnetic tape but are not in computer memory, because of limitations of memory capacity. In SCI the lack of the years 1962 and 1963 may tend to blur the picture; the years 1961 and 1964 ff. are covered. Both indexes seem to be "reasonably" up to date; our experiments did not involve this feature. What time lag exists in SCI is perhaps the unavoidable minimum for manual updating; with TIP a speed-up in updating should be possible. Coverage of the field is distinctly better for SCI than for TIP; but it is not nearly complete for either, while on the other hand the most frequently read periodicals are covered by both.

4. Advantages of a Mechanized Index

The largest citation index in the physical sciences is the one being compiled by the Institute for Scientific Information in Philadelphia. It takes 8000 pages to cover the year 1965 alone, yet this 8000 page coverage of 1600 journals in all scientific areas does not include the titles of all journals being published. (The sizes of the journals included in these 1600, however, are such that a much higher proportion of the total number of items published is included in this coverage than the number of journal titles *per se* might imply.) Such coverage will be satisfactory for some purposes, e.g., for a current awareness program, while it would probably be inadequate, e.g., for efforts to keep track of the world literature on a special subject.

Let us, however, assume that we are satisfied with this coverage as regards subject matter, and consider the problem of coverage in time. The index consists of separate quarterly volumes and cumulative annual volumes for 1961, 1964, 1965, and 1966. A similar index is to be compiled for succeeding years. Thus it will normally be necessary to look for each desired item in all the cumulative annual indexes, and separately in each quarterly supplement which has appeared since the last annual index—a total of perhaps 4–7 places. Yet, to issue supplements quarterly is hardly enough; it be currently up-to-date the supplements would have to be issued at least monthly, if not weekly. This would increase the number of places in which one must look for each item, or else cumulative indexes have to be issued more frequently. But a cumulative index providing the subject coverage of ISI and covering five years will fill about a foot of shelf space. How frequently should this much paper be thrown out and reprinted, mailed, accessioned by librarians, and physically replaced on bookshelves?

Furthermore, consider the effort of looking up an item in a list which covers a whole bookshelf. In the compilation of a bibliography, quoted above as example, a number of items have to be looked up initially. Each may be followed by several citations which have to be manually copied, examined, their references looked up, etc. All this is made prohibitively clumsy and time-consuming by the size of the index.

One might think of working with smaller indexes by having a large number of specialized indexes, each covering a certain subfield. This could work up to a point, but as specializations are made narrower, the number of citations leading from one subfield into another increases, making it necessary to look up each item in several indexes.

All these difficulties are remedied if the index is not presented in printed form but as a computer-readable record.

First, the problem of having too many supplements or having to update the master index too frequently is easily overcome in either of two ways. A computer can search several files (master and several supplements) simultaneously and use hardly more effort than in searching a single file; and it can merge the several files and produce a new updated master file, while performing one of its regular search routines, and expend hardly any additional time or effort in the process. Thus, the master file can be kept essentially up-to-date at all times; the only information items not yet incorporated into the file are those which have been acquired since the last consultation of the file, and these will be incorporated simultaneously with the next consultation.

Second, completeness of coverage is more easily approached. It is likely that the coverage of the index will have to be gradually broadened and intensified; it would be undesirable to withhold use of the index until citations from the entire desired literature have been recorded. Thus, the gradual attainment of adequate coverage will involve repeated additions to the file. In a mechanized file these can be handled easily as above.

Third, and above all, the considerable effort of manually copying relevant references out of a printed index is avoided. The computer not only finds the desired references but provides a typewritten list of authors, titles, journals, etc. Especially in the repeated back-and-forth process involved in compiling a bibliography, this is an inestimable advantage. In addition to producing a typed list of references at each stage, the computer retains the same record in its memory. The searcher can inspect the typed copy, indicate to the computer which items should be deleted (a convenient service program needs to be available for this stage), and the computer is automatically ready for the next step. Observe that on-line interaction between the questioner and the machine is desirable in this process.

These advantages are avialable, more or less, with any computer-readable citation index, regardless of the machine which is used. In our case, further benefits accrued from the special facilities of the CTSS time-sharing system of Project MAC at MIT [5], in which TIP is embedded. For example, there are simple system instructions for creating and editing files, checking them and correcting errors, printing in different formats. A single instruction will insert a change in every place where it applies. Temporary files can be created when the user has run out of permanently assigned memory space. Other system instructions monitor the operation, tell the user at his request how much time and storage space he has used etc. Different users communicate with each other by a programming scheme called "mail box," which alerts them to messages stored in the computer by one user for another; they can also, subject to an elaborate system of file protection, gain access to each other's files for data and programs. All these features were used to good advantage in our own work. There are others which, although not used by us in the present context, could be most useful in other work in citation searching. CTSS implements programming languages like COMIT which make it easy for the user to supplement the TIP instructions by programs of his own choosing for reformatting files, obtaining statistical results regarding searches, or combining citation searching with other search methods.

It might be objected that many researchers do not have easy access to computers. This problem is not as serious as it would have been a few years ago. Time sharing and remote access on large computers has passed the experimental stage and is likely to be widely available; this means that a single computer, holding the citation index in its memory, can serve a number of stations a few hundred miles away, at low cost. All the equipment the user needs is a teletypewriter or similar terminal device.

The arrangement of the index is of great importance. In the case of a printed index, searches which do not correspond to the arrangement of the index are entirely impractical; in SCI in particular, the name of the (first) author of the cited paper must be known. (The publisher of SCI has a machine-readable record of the index and could presumably perform other searches, but only at high cost.) In TIP, a variety of searches is possible, but not all are equally easy. The file is well arranged for finding (citing) papers in one or more given journals or volumes. To find all citations to a given paper, no matter when or where (within the coverage of TIP) they appear, is more costly

but by no means prohibitive. Such a search would be made easier by an inverted file; indeed, such a file could be produced easily from the main TIP file, but at present the cost of the added storage would exceed the cost of computer time saved. It is just one of the advantages of machine-readable files that they admit different types of search questions as well as reordering of the entire file, and printing of various selections from the file in various arrangements.

The user of a printed index enjoys the benefit of seeing additional related information contiguous to the entry being searched. He incurs the trouble of having to copy his answers. The computer provides printed copy, but in the case of time-shared computers the user loses time while waiting for the teletype machine to print answers. Additional waiting time can occur when the computer gets too many simultaneous inquiries.

5. Plan of Experiments

The arguments outlined above led to the conviction that citation indexing should be done by computer if at all. A series of experiments was first planned in 1964 for the purpose of becoming familiar with this technique and judging its merits. At that time the TIP file at MIT was the only conveniently accessible citation index in computer-readable form. Being limited to physics, it seemed a logical choice for experiments to be conducted by the National Bureau of Standards.

The set of *citing* papers in the TIP file consists of all papers in a small selected group of physics journals, numbering about 20 in 1964 and since expanded to over 30. It includes all of the most important physics journals in the United States, and a sampling of foreign journals. In the case of Russian journals the English translation is used. For most of these journals, all volumes beginning with 1963 are included. Table 1 presents a recent listing of the TIP "library" of citing journals.

The set of *cited* papers consists of most, but not all, the papers cited in the citing papers. Included are those, and only those, papers appearing in a list of about 250 journals. There is no time limit; all volumes are covered. All citing journals, of course, are among the cited journals, including the volumes earlier than 1963. Excluded from the list of cited papers are all references to journals other than the 250 or so "cited journals" as well as all references to the nonperiodical literature.

In addition to the file itself, TIP offers a computer program for retrieving information from the file. The file and the program are part of the CTSS time-sharing system at Project MAC [5]. The program can retrieve items according to several criteria, such as papers by a given author, papers containing certain expressions in their title; the two criteria most important for our purposes are

(a) finding citations to a given paper,

(b) finding papers which have at least one citation in common with a given paper.

We had initially planned to concentrate on experiments with (b); gradually we had to recognize the need for conducting a large part of the investigation by means of (a). Obviously (b), which is known as "bibliographic coupling" or "share bibliography" searching, is a special case of (a); a request of type (b) can be executed by finding all citations in the given paper and then finding citations *to* any of them. In (a) the given paper must be in one of the 250 "cited journals," in (b) it must be in the "library," i.e., it must be in one of the 30 "citing journals" since 1963.

In the spring of 1964 we began by enlisting the participation of a number of physicists at the National Bureau of Standards. There were seven individuals, plus one close-knit group of several people. They represent a cross section of research in physics at the Bureau, are active in creative work and at the same time high enough in the administration so that their judgment of our experiment would carry weight. We attempted to make the least possible demands on the participants' time. Each of these persons supplied a list of his publications. Their size may be seen in table 1. Our first intent was to attempt bibliographic coupling, i.e., search for papers which share references with those given, separately for each of the eight bibliographies.

Since at that time long-distance access to the MAC computer was not practical, the original plan was to have the computer runs carried out by the TIP group at MIT. After some time it became clear that this would not be feasible, and we began to look for remote access to the computer.

Table 1

LIBRARY

THE DATE IS 01/17/67
THE VOLUMES AVIALABLE TODAY ARE . . .

ANNALS OF PHYSICS
J384–ANNPHY–ANN PHYS
V 26–39
APPLIED PHYSICS LETTERS
J646–APPLET–APPL PHYS LETTERS
V 3–9
CANADIAN JOURNAL OF PHYSICS
J55–PHYCAN–CAN J PHYS
V 42–44
DISCUSSIONS OF THE FARADAY SOCIETY
J153–DISFAR
V 40
HELVETICA PHYSICA ACTA
J43–PHYHEL–HELV PHYS ACTA
V 37–39
INDIAN JOURNAL OF PHYSICS
J164–INDJPH–IND J PHYS
V 38–39
ETP LETTERS
J821–JETLET–JETP LETTERS
V 1–4
JAPANESE JOURNAL OF APPLIED PHYSICS
J612–PHAPJA–JAPAN J APPL PHYS
V 3–5
JOURNAL OF APPLIED PHYSICS
J11–PHYAPP–J APPL PHYS
V 35–37
JOURNAL OF CHEMICAL PHYSICS
J12–JCHEPH–J CHEM PHYS
V 40–45
JOURNAL OF CHEMICAL PHYSICS SUPPLEMENT
J842–JCHEPS
V 43
JOURNAL OF MATHEMATICAL PHYSICS
J227–MATHPH–J MATH PHYS
V 6–7
JOURNAL OF THE OPTICAL SOCIETY OF AMERICA
J45–JOPSOC
V 55–56
JOURNAL OF THE PHYSICAL SOCIETY OF JAPAN
J80–PHYSOJ–J PHYS SOC JAPAN
V 19–21
IL NUOVO CIMENTO
J17–NUOCIM–NUOVO CIMENTO
V 31–45
IL NUOVO CIMENTO SERIES B
J841–NUOCIB
V 40–42
IL NUOVO CIMENTO SUPPLEMENT
J843–NUOSUP
V 3
MOLECULAR PHYSICS
J160–MOLPHY
V 9–11
NUCLEAR PHYSICS
J682–NUCPHY–NUC PHYS
V 50–85
PHILOSOPHICAL MAGAZINE
J28–FILMAG
V 9–14
PHYSICA
J21–HYSICA–PHYSICA
V 30–32
PHYSICS LETTERS
J49–PHYLET–PHYS LETTERS
V 8–23
THE PHYSICS OF FLUIDS
J799–PHYFLU–PHYS FLUIDS
V 7–9
PHYSICAL REVIEW
J1–PHYREV–PHYS REV
V 133–150
PHYSICAL REVIEW LETTERS
J41–PHYRET–PHYS REV LETTERS
V 12–17
PHYSICAL REVIEW, SERIES B
J199–PHYREB–PHYS REV B
V 133–140
PROCEEDINGS OF THE PHYSICAL SOCIETY (LONDON)
J3–PHYPRO–PROC PHYS SOC
V 83–89
PROCEEDINGS OF THE ROYAL SOCIETY
J23–PROCSO
V 283–294
PROGRESS OF THEORETICAL PHYSICS (KYOTO)
J29–PROPHJ–PROGR THEORET PHYS
V 31–36
PROGRESS OF THEORETICAL PHYSICS SUPPLEMENT
J840–PROPHS
V 34–965
SOVIET JOURNAL OF NUCLEAR PHYSICS
J825–SOVJNP–SOVIET J NUC PHYS
V 1–3
SOVIET PHYSICS–JETP
J669–SPJETP–SOVIET PHYS JETP
V 18–23
SOVIET PHYSICS–SOLID STATE
J310–SPSOLS–SOVIET PHYS SOLID STATE
V 6–8
SOVIET PHYSICS–TECHNICAL PHYSICS
J790–SPTPHY–SOVIET PHYS TECH PHYS
V 9–11

END OF LIBRARY

Shortly thereafter the TIP file was temporarily removed from the MAC computer to allow for remodeling the system. It was not until November of 1965 that we could run the first trials from remote consoles at NBS in Gaithersburg, Md. After an interruption of a few months these experiments were resumed in the summer of 1966, and a number of trial runs have been made since then.

Meanwhile our bibliographies were 1½ years old and contained few items of 1963 or later; citing papers published before 1963, originally included in the TIP file, had been removed from the file. A meaningful search for shared references was possible for only one author, whose bibliography included 7 papers in 1963 and 1964 in one library journal. We searched the last three years of the same journal for shared references with one of these and found 20 papers. The author decided (by inspection of the titles and authors' names) that about 13 of the 20 would be relevant to his field of interest—a high percentage, considering that any paper was "found" if it had even one

reference in common with one of his own papers. It would have been interesting to see whether and how much the "relevance ratio" improves if the search is limited to papers sharing 2, 3, . . . references with the source item; but this would require a larger sample, and programming of special instructions in CTSS outside the TIP system. Nor could we obtain any good information on the "recall ratio" i.e., on how many of the potentially relevant papers were found and how many were missed by the search. Before we had a chance to extend the search to all seven eligible papers and to additional journals, our access to the computer was temporarily interrupted.

When we were able to resume work in the summer of 1966, we decided to follow two lines of approach. One was to search systematically for citations *to* the eight sample bibliographies, in order to obtain comparable data for different areas of physics and some feel for the relevance of references so obtained. The other was to use any handy opportunity to explore the degree of completeness of literature lists obtained through citation indexing, perhaps iterated, and bibliographic coupling; such opportunities are infrequent and have to be used as they arise. A hoped-for by-product of both approaches was to gain experience with remote computer access.

6. Relevance

Some facts about the eight bibliographies of NBS authors used in this study are summarized in table 1. There were a total of 363 references, of which 297 were to publications in 1940 or later. Of this latter group, 176 were to papers in the 250 "cited journals" covered by TIP. The other references were either to papers in other journals or to non-journal items (books, reports, proceedings, etc.). The TIP library, i.e., the set of citing papers recorded in TIP, was searched for references to each of the 8 groups of papers making up this list of 176. At the time of these searches the TIP library covered about 25 journals mostly for the years 1963–1965, in some cases also part of 1966. As might be expected, the results vary greatly from author to author. The TIP library consists mostly of journals heavily oriented toward modern fields of physics, such as nuclear and solid state physics. This is one reason for the relatively high number of citations to the papers of authors B, C, E, and H.

Other factors come into the picture too. The absence of citations to papers by author F reflects not only the fact that his fields of interest are not well covered by the TIP library, but also the fact that they are older than the others; 7 of the 11 papers date from before 1950. It is known from other studies of citation indexing that most citations come in the first five years after the appearance of the cited paper.

The purpose of this group of searches was to judge the relevance of literature obtained by citation indexing. No precise results could be expected, because the concept of relevance is so vague. Thus there seemed to be no need to spend great effort in determining the degree of relevance of retrieved papers, especially in view of our desire to minimize the inconvenience to participating authors. These authors were merely shown the retrieved lists (titles and authors of citing papers) and were asked for a quick judgment of whether these papers were pertinent to their field of interest. The answer was affirmative in a large majority of cases, as indicated in the last column of table 2. Uncertainties arose rarely from inability to judge the content of a retrieved paper on the basis of its title and author(s) alone; they arose commonly from judgments like "moderately interesting" or "slightly interesting" and from the lack of consistency among the judging authors in using such terms.

The retrieved references include some papers by the cited authors themselves, in cases where they publish in one of the 25 journals of the TIP library and reference their own earlier papers. This is not a major factor; there is only one such paper by author B, 4 by author C, 3 by D and 6 by the group of authors represented by H (including, of course, mutual references of these authors to each other).

Since all authors are affiliated with the National Bureau of Standards, it may be remarked parenthetically that the NBS Journal of Research is not among the 250 "cited journals" of TIP; thus all papers published by the authors in that journal had to be omitted from the study. Another

TABLE 2. *Citation searches to publications of eight solicited authors*

Author	Field	Number of items in bibliography since 1940	Number in cited file	Number retrieved in citation search	Relevant
A	Cryogenics	52	31	11	7
B	Photonuclear reactions	29	18	44	Many
C	Molecular spectroscopy and statistical mechanics.	53	43	53	50
D	Molecular spectroscopy	49	47	68	60
E	Neutron reactions	20	[c] 6	9	9
F	Metrology and geophysics	[b] 58	11	0	
G	Metrology and electricity	8	2	1	0
H [a]	Solid state physics	28	18	43	Many
	Total	297	176	229	

[a] Group bibliography.

[b] Does not include 80 publications prior to 1940.

[c] Excludes a number of older papers in "cited file" but omitted from search because somewhat different field.

curiosity concerns one paper retrieved among the references to author A, which the author judged totally irrelevant; a follow-up showed that the paper made reference, not to a paper by author A, but to another paper starting on the same page in the Physical Review as one of author A's papers. Such papers are indistinguishable in the TIP system if they occur only as cited papers; this is only a minor annoyance here, since it causes only a small number of false drops; it would be more serious in an index including letters to the editor and other short items.

7. Completeness

It is quite difficult to determine how completely a procedure—for instance a particular request to a citation index—recalls all of the desired literature.[3] The difficulty lies in finding a control procedure which can be relied upon to produce complete recall. Usually a painstaking literature search by a subject matter specialist is the only method. We availed ourselves of a few opportunities in which such searches had been made or in which we could persuade a scientist to make them. In some cases it turned out after the fact that, for some reason or other, no valid inferences could be drawn; we shall nevertheless mention in the following even these unsuccessful attempts.

(a) In our first trial we were hoping, while examining recall, also to explore the usefulness of citation indexing for data retrieval—the primary problem which has caused us at NBS to take an interest in this subject. We chose NBS Circular 500, "Selected Values of Chemical Thermodynamic Properties," first published in 1952 and now coming out in a new edition; more specifically we selected the sections dealing with the elements Si, Ge, Sn, Pb, Ga, In, Tl (and their compounds with those elements preceding them in the standard order of arrangement). The first edition contains an extensive bibliography for each of these seven groups. It was our plan to look for citations to items in this older bibliography, and compare the list so obtained with the list of recent publications actually used by the compilers of Circular 500 in the new edition.

In the first edition of Circular 500, there were about 270 references in the seven sections included in our study, but only 123 of them were to the 250 "cited journals" of TIP; the others were references either to the nonperiodical literature, or to journals not included in the TIP list of cited journals. We then searched the entire TIP file of 25 citing journals for papers citing any of

[3] The term "recall ratio" is commonly used for the ratio between the number of items retrieved by the tested procedure to the total number of items that one would wish to retrieve. This is in contradistinction to the "relevance ratio" discussed in the preceding section.

these 123 papers. (This required some maneuvering with tapes and specially created files; the TIP System does not easily accommodate searches through many journals for finding references to many different papers, for customers having only a small amount of computer storage allotted for their use.) In the end, somewhat to our surprise, we found only six such references. In retrospect the reason for this disappointing result seems to be that the subject of Circular 500—thermodynamic properties of materials—is not usually represented in the citing journals covered by TIP. The latter focus on the mainstream of modern physics. Recent papers on the more classical subjects, such as thermodynamics, would have to be looked for in a different set of journals.

(b) We then turned our attention to a field which is strongly represented in TIP, nuclear physics. From a nuclear physicist at NBS ("author J") we obtained five "fundamental references" on the subject of neutron scattering. They are:

Phys. Rev. **55,** 190, W. E. Lamb, Jr., Capture of neutrons by atoms in a crystal (1939).

Phys. Rev. **94,** 1228, G. C. Wick, The scattering of neutrons by systems containing light nuclei (1954).

Phys. Rev. **95,** 249, L. Hove, Correlations in space and time and Born approximation scattering systems of interacting particles (1954).

Phys. Rev. **101,** 118, A. C. Zemach and R. J. Glauber, Dynamics of neutron scattering by molecules (1956).

Phys. Rev. **110,** 999, G. H. Vineyard, Scattering of slow neutrons by a liquid (1958).

Searching the entire TIP library for papers citing one of the five basic ones, we obtained 93 papers. By inspecting the titles and authors' names of the referenced papers, author J concluded that all but about 15 were relevant. To keep further work within manageable limits, he selected 16 out of the 78 relevant papers; these pertain to a narrower subject, broadening of neutron resonance lines. With these we searched for papers with shared references, limiting the search to five Soviet journals (a total of 15 volumes). This resulted in a list of 80 papers.

As was to be expected, a majority of them were not relevant; our aim was to get high recall, even at the expense of high admixture of irrelevant papers.

To test the completeness of recall, author J kindly examined two of the 15 volumes searched, namely, volumes 18 and 20 of the English translation of Soviet Physics—Journal of Experimental and Theoretical Physics (JETP). Of the 80 papers found in the TIP search, 22 were in these volumes, including nine relevant, one marginal, 12 not relevant to the topic (broadening of resonance lines). By looking only at the Tables of Contents of the two volumes (i.e., authors and titles), author J spotted 19 potentially relevant papers. Closer examination of the papers themselves showed that six of the 19 were not relevant and three were marginal, leaving only 10 clearly relevant. That is to say, the precision of a human search using authors and titles only was in this instance not much better that of the TIP search. Even more surprising was the low degree of overlap between the two searches. Only six papers appeared in both searches; five of these were relevant ones; one was irrelevant, despite the fact that its title had looked pertinent and that it had one citation in common with each of two previously found papers in the field. The following table summarizes the result.

	Search for papers on neutron resonance broadening				
	Found by author J			Not found by author J	Total
	Relevant	Marginal	Not rel.		
Found by TIP: Relevant	5	*	*	4	9
Found by TIP: Marginal	*	0	*	1	1
Found by TIP: Not rel.	*	*	1	11	12
Not found by TIP	5	3	5	?	13+
Total	10	3	6	16+	

Not only was the relevance ratio of author J not much better than that of the TIP search, but his recall ratio was not much better; he missed four relevant and one marginal paper found by TIP, while TIP missed five relevant and three marginal papers found by author J. It is true that the omissions of author J were not entirely due to misleading titles, but were in part caused by the rapidity of scanning the Tables of Contents; but it is legitimate to charge the manual search method with being tiring and therefore conducive to error.

(c) In section 6 we mentioned 44 papers retrieved in a search for citations to the publications of author B. It happens that this author maintains a bibliography intended to be reasonably complete on photonuclear reactions and related phenomena. We recognized that this bibliography could serve as a control for our purposes without requiring any great additional effort on the part of the author. To investigate how quickly we could advance toward a complete bibliography, we decided to continue from the 44 citing papers retrieved earlier, by searching the library for papers which share at least one reference with one of them. This is equivalent to obtaining all papers cited by the 44, and then obtain further citations to these cited papers. (Because of minor technicalities three of the 44 papers were omitted from the search.)[4]

The author's file consists almost entirely of papers from five journals—*Nuclear Physics*, *Physical Review*, *Phys. Rev. Letters*, *Physics Letters*, and *Soviet Physics—JETP*. At the time of this study there were 235 such papers. In addition there were 25 papers scattered among other journals, and 12 non-journal items. Of the 235, only 69 were from 1963 or later, the others were thus too old to be retrieved from the TIP library. Our plan was to see how completely these 69 papers could be retrieved by a few steps of citation indexing. Table 3 shows the results of the search. To save time, only those volumes of the five journals were searched in the TIP library which contained articles on author B's list. These volumes contained a total of 5,845 papers, of which 1,074 were "retrieved" by the criterion that they share at least one reference with one of 41 papers citing author B. Most of these 1,074 were not relevant to photonuclear reactions; but included among them were 57 which were relevant, as evidenced by the fact that they were listed in author B's bibliographic file. Thus 57 out of 69 possible papers were retrieved in one step of bibliographic coupling, starting from a base of 41 papers which undoubtedly were not an optimal base.

Having thus learned that bibliographic coupling with these 41 papers was sufficient to retrieve most papers of interest, we applied the same search to a number of other journals in the TIP library; journals which author B was not likely to consult because they do not emphasize nuclear physics. The results are shown in table 3b. Of the less than 5,000 papers in these journals, 259 satisfied the search criterion. Again most of them were not relevant, but author B found three papers among them which were of interest, and which had not previously come to his attention. This points up one of the more promising applications of citation indexing: to search "low-yield journals" which are not likely to contain many items if interest, which an author would therefore not normally look at, and select from them a manageable list of papers which still contains most of the interesting items.

(d) Author E, in addition to supplying the references listed in table 2, had also given us, at our request, a list of five papers by other authors, which he considered as characteristic of his field of interest. These were:

Fluctuations in partial radiation widths of U^{239}, H. E. Jackson, Phys. Rev. **134,** B931.

Neutron resonance spectroscopy III Th^{232} U^{239}, J. B. Garg, J. Rainwater, J. S. Petersen, and W. H. Havens, Jr., Phys. Rev. **134,** B985.

Theory of radiative capture in the resonance region, A. M. Lane and J. E. Lynn, Nuclear Physics **17,** 563 (1960).

Anomalous radiative capture, Lane and Lynn, Nuclear Physics **17,** 586 (1960).

Parameters and gamma ray spectra, R. T. Carpenter and L. M. Bollinger, Nuclear Physics **21,** 66 (1960).

[4] This search would have been rather slow if done by remote access. The authors thank Mr. W. Mathews of MIT for running it on the computer.

TABLE 3. *Search for papers sharing citations with any of 41 papers citing author B*

a. Journals previously scanned by author

Journal	Volumes searched	Number of papers			
		Searched	Retrieved	Relevant	Known to author
Phys. Rev.	B133–B140	1,785	474	7	8
Phys. Rev.	141, 143, 149	577	73	7	7
Nuclear Phys.	51–54, 56–57, 59–60, 63–64, 70, 74–76.	781	292	29	35
Sov. Phys. JETP	19	266	11	0	2
Phys. Ltrs.	8–9, 11–13, 16–19	1,788	183	12	14
Phys. Rev. Ltrs.	12, 15	648	41	2	3
	Total	5,845	1,074	57	69

b. Low-yield journals

Appl. Phys. Ltrs.	3–9	899	0		
Melv. Phys. Acta	37–39	238	14		
Prog. Th. Phys. (Kyoto)	31–36	400	40		
Nuovo Cim.	31–45	1,151	65		
Canad. J. Phys.	42–44	476	30		
Physica	30–32	437	15		
Sov. J. Nuc. Phys.	1–3	462	64		
Proc. Phys. Soc. Lond.	83–89	765	31		
	Total	4,828	259	3	0

A search of the TIP library for citations to these papers brought forth eight papers, including three in Russian journals. All were judged highly relevant to the field, and the discovery of the Russian papers was a welcome bonus to the author, but the small volume of the result was disappointing.

(e) A physicist at the National Bureau of Standards ("author K") needed a bibliography on computation of molecular wave functions, and was persuaded to attempt use of the TIP file in parallel with a conventional approach. He supplied a list of 33 authors and of the journals in which they habitually publish—two or three for each author, mostly, *J. Chem. Phys.* and *J. Mol. Phys.* A search of these journals in TIP, specifying the authors, gave 133 papers. The same search was performed by an assistant reading through the tables of contents of the journals. Comparison of the results showed that (1) the search in TIP missed three papers, two because the author's name was misspelled in the computer file and one because of a confusion on input; (2) the human assistant overlooked several papers; (3) the 133 papers produced by TIP included about 20 by authors with names similar to, but not identical with, those requested (usually different initials), because the input was not specific enough. This, of course, is only a minor annoyance, less serious than omission of a desired reference.

We then searched the TIP record of *J. Chem. Phys.* and *Mol. Phys.* for citations to any of 129 papers found in the first step, specifically, all those of the 133 which appeared in these two journals, omitting only four papers from other journals. The 20 or so false drops of the first step were included because they had not been discovered at the time of this search. The result was a list of 167 papers, of which 99 were judged relevant by author K.

(f) The search conducted for author K gave as a byproduct a comparison between manual and computer searching. Another experiment was made expressly for this purpose; it consisted in duplicating by means of the Science Citation Index [4] one of the searches previously made in TIP. We caution against considering this as a comparison between SCI and TIP for completeness; a meaningful comparison for this purpose would require a far larger sample than the one used here. We were interested in ease and convenience of the processes, and these can be judged to some extent even from a single attempt. As it turned out, however, the experiment revealed more about peculiarities of the two indexes used than about the difference between manual and machine methods in general.

The search for references to author B, reported in section 6 above, started with 29 publications by B and resulted in 44 citations to them. Of these, 26 appeared in 1964. We searched manually in SCI for 1964 and found 25 references to B. Of the two sets of references, 21 overlapped. SCI missed five because the citing journals (*Phys. Letters, Sov. J. Exp. & Theor. Phys.*) are not covered by SCI. TIP missed four citations, of which one is to a cited journal not covered by TIP (*J. Res. Nat. Bur. Standards*), three are to citing journals not in the TIP Library (*Rev. Mod. Phys., Zeitschr. f. Phys., Atom. En. Rev.*). As for convenience, compare (1) walking to the library in adjacent building, starting to search, finding an unanticipated need for additional information, having to walk back to one's office to locate it, and then once more to the library; and (2) walking down two flights of stairs to the nearest teletype, dialing the computer, finding all lines busy, repeating this a little later, and finally deciding to run the search late at night when the computer is less in demand. Once connection is made, the computer needs only a few minutes of main frame time, but these are spread over 1–2 hours of real time; at the end of this time we have a neat printed list of all desired citations, 1963–1965. With SCI, we quickly located author B in the 1964 volumes and copied 18 citations; realized that this was incomplete; remembered that SCI lists only first authors; fetched B's list of publications; located all papers where B appears as second author; noted the first author (mostly the same on all papers—call him L); located author L in the 1964 SCI; picked out, with some effort, citations to those of L's papers on which B was co-author (this requires going back to B's publications list each time, since B's name does not appear in SCI with these papers) and finally copying seven references to these papers. After spending about 1½ hours in the library, we now had the 1964 citations and not enough patience to repeat the process for other years. Comparison of the two sets of citations revealed that they were completely explained by the different coverage of the two indexes, so that there appeared to be no erroneous omissions.

8. Conclusions for the User

What does the user get out of citation searches? It depends on what he has got out of other search methods, on his field of interest, and on the purpose of his search.

A first fact which emerges from our experiments is that papers which cite a given author are usually in the author's own field of work, more so than one might have expected. Papers in other fields are a small minority. Many of the papers found in these searches were already known to the cited authors, but most authors found at least a few papers—typically perhaps 25 percent—which were new to them. Authors who keep reasonably complete bibliographies in their fields are not likely to find much of value in such a search; in our sample, author B was in this class. But an author who, like most scientists, habitually scans only a few journals in his field and otherwise relies on personal contacts for keeping informed, is likely to find a number of references that are new to him.

The results of such a search for citations to one author's papers are quite incomplete; that is, there are usually many papers in the literature which are of interest to the author even though they do not cite his writings. One can obtain more complete coverage by an iterative process, in particular, by searching for papers which share references with papers in a given list. (This list may consist of the author's papers, or better, may include some or all of the references cited in

his own paper.) Here the results will depend strongly on the size of the starting list; in our sample, starting with half a dozen papers gives few results, starting with about 40 gives over 80 percent coverage. This high coverage is bought at the price of a very large admixture of irrelevant papers. The author has to plow through a large number of retrieved papers to find the few that are of interest to him. Nevertheless the process is not entirely useless. Even if the retrieved papers constitute, say, 15 percent of the search range (as they do in table 3), the author's work in looking for relevant papers has been reduced by 85 percent. The method appears especially promising if applied to "low-yield" journals, i.e., those in which only a small fraction of all papers is in the author's field, and which the author would therefore normally not consult.

Both kinds of searches seem to be successful enough to be used as supplements to other methods of literature retrieval, but not good enough to be relied upon as the sole means, or even a principal means, by which scientists are kept informed.

It is plausible that the performance of shared-reference searches could be improved by enlarging the starting list of papers and at the same time tightening the search conditions to require two or more shared references. Unfortunately it was not possible to explore this conjecture in the course of our program. In the TIP system such a search must be conducted by first searching for all shared references and then weeding out all papers with only one shared reference, so as to retain only those with multiple shared references. This would have to be done with a large list of starting papers, but even the 41 papers of section 7c above were almost beyond the limits of machine time and memory available to us.

Sitting at a console, keying questions into it and seeing results typed out has a number of advantages which are worth listing here. We were rarely able to anticipate the volume of output generated by a question. It is well to feel one's way, search one volume at first, gradually increase the search range. When finding high yields in some journals, low ones in others, one can then combine several low-yield journals into one search, subdivide a single high-yield journal into several searches. Similarly, it is economical to combine a number of questions into a single search, to save computer time. It is then better to store the answers and print them on a subsequent run, rather than print at once, in order to separate the answers pertaining to the different questions. But this runs into the limitation of memory available to individual users of the MAC computer, and therefore is again best done by on-line operation, where one can stop just before having exhausted one's memory quota. After much experience, these precautions could be anticipated and incorporated into batch-processed computer runs, but many scientists are likely to use citation searching only occasionally, without ever becoming expert at it.

In our experience, in one hour of time spent at the console one gets anywhere from less than 1 to 10 or 15 minutes of main frame computing time; the average might be 2 minutes.[5] The commercial value of 2 minutes on a large computer is about $20, the cost of a one-hour telephone or teletype connection is of the same order of magnitude. We believe that the greater convenience and efficiency afforded by on-line operation is well worth the added cost.

We have already mentioned certain limitations which are peculiar to the TIP file, rather than to the method in general. The file covers some areas of physics poorly, other areas very well, but not completely. In time it covers three or four years. It omits all citations to the non-journal literature and to some less frequently used journals. The first of these limitations was deliberately imposed because of the experimental nature of the entire TIP project. The second is due to memory limitation of the MAC computer. The third is caused merely by the encoding method chosen—three decimal digits to represent a journal—and could be most easily overcome.

Despite the limited file size, the time taken for searching is fairly long. The TIP manual states that one search of the entire file takes three minutes of main frame time. Since that manual was written, the file has been enlarged, so that the search time has become longer.

In a dozen searches which we ran in different parts of the file, the computer searched an average of 100 papers per second; the speeds ranged from 40 to 160 papers per second, with a

[5] These numbers should not be generalized without scrutiny; they are peculiar to the time-sharing system used, and especially to its scheduling algorithm.

standard deviation (rms) of 40. It would probably take 5 to 6 minutes of main frame time to search through the present file for a single question, at a cost (if done commercially) of $50 to 75, plus a similar amount for phone time if done at long distance. Furthermore, we have found that almost invariably the machine time is somewhat longer than the nominal time given by the TIP manual, presumably because of some housekeeping operations. Finally, the nominal time is for single questions. It increases only slightly if a few questions are processed simultaneously, but it becomes several times as long for batches of 40 or 50 questions. It seems likely to us that the computer time could be substantially reduced if search programs were written with this goal in mind; as is appropriate for a research project, the original search programs were written for flexibility rather than for economy of computer time. Further time savings could undoubtedly be realized if the file were kept in several different arrangements, including one sorted on cited papers like the ISI Science Citation Index. But whether the resulting economies would offset the increased cost of storage is a question we are unable to answer.

9. Some Extrapolations

In describing our experiments with the TIP system we have noted the usefulness of the CTSS remote access time sharing system in which TIP is imbedded. The usefulness of the TIP system as one for manipulating citation index data is considerably enhanced by the properties of the CTSS system. However, in a broader sense we may view the set of experiments above as a special case of a more elaborate system for manipulating scientific information, whose eventual development we may anticipate by extrapolating from our experience with the experiments described above.

It should be noted at the outset that the notion of a citation index is itself a derivative from the historical development of conventional publication media. If we are willing, however, to accept the technological fact that scientific information communication can be mediated by a remote access computer then it becomes possible to consider a whole new class of services that such a remote access computer mediated communications system can achieve. The main arguments against such services are economic in nature. As to whether or not such eventualities will actually occur—whether in the near or far future—is more a question of economics than of technological possibility.

One such possibility which we have already explored and mentioned above is the rather straightforward one of communicating conventional mail type of information. In a system such as CTSS, it is possible to compose memoranda and to mail them to other users. The other users receive a notice of the existence of such mail whenever they enter the system, usually for other computing purposes. A modest extension of this capability allows the initiative to be taken by the system to call the user and notify him of the existence of mail. A still further extension of such capability allows its use as a distribution system for documents like reports and others of a nature less formal than conventional publications. Such a distribution system is of course entirely under the control of the mediating computer programs. Thus the possibility of differential distribution lists as a function of time and subject content become possible.

A much more important possibility is that of differential distribution of documents through a remote computer system in which the change from one time to the next is in the contents of the documents themselves rather than in the distribution list for the documents. A document, for example, may change in time as a function of use, because of the addition of editorial corrections, or the addition of comments that may be considered the equivalent of marginal notes by readers. In certain special cases these may be allowed to update the master document. Again access to the updating function to the document itself may be controlled by the author or some more complicated agency, under his control. The most important point to note here is that the contents of the document being manipulated within such a system are subject to extensive change by a network of readers and potential readers whose changes are themselves partly under the control of the author of the document.

On the question of economics of such a system the only observation worth mentioning at this point is that such a system cannot achieve practicality until the number of interconnected users becomes sufficiently large that the set of potential readers of documents may be considered to be largely included within the set of users of the system. For specialized classes of users this technological possibility is perhaps economically realizable now. For general scientific documents this of course is not yet the case.

We have thus far unnecessarily been assuming implicitly that the information to be communicated within such a remote access distributed network of users is like conventional documents. But even if we wish to preserve the archival function of conventional publication media we need neither preserve the passive nature of the documents nor their relative immutability. Our notion of a less passive more extended document might include one containing the description of procedures, like computer programs or process control procedures for example, which need not be read in a conventional sense at all but merely called by other programs and used, without the occurrence of an intermediate process of reading and understanding, by some individual person. Programs in a system like the CTSS system are conventionally used in just such a fashion. Most of the programs that a user invokes he never reads. Instead he obtains some form of certification (in this case usually informal) as to the validity of the process which he is using, and then proceeds without further inspection of the document at all.

Thus "quasi-documents" in such a system are active in the sense that they directly influence subsequent processing of information without the intermediating process of human consumption of the quasi-documents. Such quasi-documents are also less immutable as a function of time. The situation can be so arranged that when one calls upon a quasi-document for inspection only the latest version will be furnished by the system. The current version distributed will be the latest one with all the changes up till the point of calling of the quasi-document from the system. The historian or others interested in the archives may in such a case generally get access to original documents or prior versions of such a quasi-document where the archiving function exploits the variable kinds of access in such a system, older documents having been superseded by archiving them in less accessible kinds of storage like magnetic tape.

Since we are willing in these speculative comments to consider the possibility of extensive modification of the usual scientific publication process we might also briefly consider the possibility of largely avoiding this process altogether in certain cases. We have in mind the possibility of allowing the scientific information that ordinarily results in publication to reside implicitly in the authors of such documents without necessarily receiving any external form until called upon for use by the system. The way this could be achieved is in a very large system with users who may be called upon, on the initiative of the system, to serve its purposes of information access. Users whose interests and competence profiles are stored in such a system might be addressed by the system when it needs information from those users of appropriate expertise who are in consultant mode at that moment. The "consultants" would "publish" their information when it is needed and otherwise it would not be recorded. One can imagine such a system responding rapidly to scientific information needs of the moment, with of course the concomitant disadvantage of the loss to the publication process of those kinds of scientific information which anticipate future needs rather than respond to them. The solution to this problem is of course to include both possibilities within such a system. But for the evanescent needs for certain kinds of scientific information the possibility of a remote access system being helped by consultants on line who supply information when it is needed, by the machine, should not be entirely ignored.

Notice that such a system is the dual of a conventional time sharing system, which we might more profitably view as a machine information distribution system, aided by people, rather than people aided by such a machine. Such a "man-aided computer" can offer some of the advantages in use of human efforts that a conventional time sharing system offers in the utilization of machine capabilities. We are thus considering the more complex kinds of scheduling algorithms for people and their scientifically productive efforts, that might be possible in such a system, in which access to people and their information is mediated by a computer with its elaborate scheduling capa-

bilities, just as now we have access to the computer mediated by that same kind of scheduling capability.

The above speculative comments have been inspired by the existence within the MAC CTSS system of nascent versions of most of these proposals. We have raised the issues largely because in most of these areas no technological limitation prevents us from exploiting these possibilities. Rather the demand by a large set of users for such capabilities at a level of economic feasibility is what is more likely to influence the ultimate existence of such capabilities, within a computer mediated scientific information system. Thus if potential users can begin thinking about such possibilities the ultimate economic realization of them can be speeded up.

10. References

[1] Brown, Sanborn C., A bibliographic search by computer, Physics Today, **19,** No. 5, 59 (May 1966).

[2] Kessler, M. M., The M.I.T. Technical Information Project, Physics Today, **18,** No. 3, 28 (March 1965).

[3] Pyke, Thomas N., Jr., Time-shared computer systems. Advances in Computers, **8,** 1 (Academic Press, New York).

[4] Garfield, E., Science Citation Index—a new dimension in indexing, Science, **144,** No. 3619, 649 (May 8, 1964).

[5] Corbató, F. J., et al., The Compatible Time-Sharing System (MIT Press, Cambridge, Mass., 1963).

[6] Garfield, E., and I. H. Scher, ASCA (Automatic Subject Citation Alert), A new personalized current awareness service. Amer. Behavioral Scientist, **10,** issue 5, p. 29 (1967).

(Paper 72B1–260)

JOURNAL OF RESEARCH of the National Bureau of Standards—B. Mathematical Sciences
Vol. 72B, No. 1, January–March 1968

Simple Analytic Expressions for the Total Born Approximation Cross Section for Pair Production in a Coulomb Field

L. C. Maximon

Institute for Basic Standards, National Bureau of Standards, Washington, D.C. 20234

(January 9, 1968)

The total Born approximation cross section for pair production in a coulomb field given originally by Racah is used to derive two simple and rapidly convergent analytic expansions for this cross section, one valid for high energies, k, of the incident photon, the other for energies near the threshold. For $k > 4mc^2$ the fractional error involved in using the first four terms in the high energy expansion is $< 4.4 \times 10^{-3}$. For $k < 4\ mc^2$ the fractional error committed in using the first five terms of the low energy expansion is $< 1.1 \times 10^{-4}$. The leading terms in these expansions are the well known high energy and low energy limits of this cross section, respectively.

Key Words: Born approximation, coulomb field, moderate energy cross section, pair production, Racah cross section, total photon cross section.

The cross section for the production of an electron-positron pair in the field of an unscreened Coulomb potential $V = -Ze^2/r$ was first given in first Born approximation in a number of papers nearly thirty five years ago by W. Heitler and F. Sauter [1],[1] H. Bethe and W. Heitler [2, 3], and G. Racah [4]. References 1, 2, and 3 give this cross section, differential in energy but integrated over all particle directions, without any approximation in the energy [5] as well as in a form valid when the energy of each of the pair particles is extremely relativistic (E.R.) [6], ($\epsilon_1 \gg 1$, $\epsilon_2 > 1$):

$$\frac{d\sigma}{d\epsilon_1} = 4\bar{\phi}\,\frac{\epsilon_1^2 + \epsilon_2^2 + \frac{2}{3}\,\epsilon_1\epsilon_2}{k^3}\left(\ln\frac{2\epsilon_1\epsilon_2}{k} - \frac{1}{2}\right) \qquad \text{(E.R.)} \qquad (1)$$

where

$$\bar{\phi} = \frac{e^2}{\hbar c}\left(\frac{Ze^2}{mc^2}\right)^2 = Z^2 \cdot 5.7938 \times 10^{-28}\ \text{cm}^2. \qquad (2)$$

and ϵ_1, ϵ_2, k are the energies of the positron, electron and photon respectively, in units of mc^2. References 2 and 3 give the total cross section (eq (1) integrated over ϵ_1), but only in the extreme relativistic limit ($k \gg 1$):

$$\sigma = \bar{\phi}\left(\frac{28}{9}\ln 2k - \frac{218}{27}\right). \qquad \text{(E.R.)} \qquad (3)$$

Only in the papers by Racah can one find an expression for the total cross section involving no high energy approximations. Unfortunately, this expression involves indefinite integrals over elliptic integrals, so that it is quite inconvenient for obtaining numerical values of the total cross section. In fact, for this purpose it is equally simple to integrate directly, numerically, the differential cross section [5] in which no high energy approximations have been made. However, both

[1] Figures in brackets indicate the literature references at the end of this paper.

289-930 OL-68—6

for numerical evaluation and for an understanding of the analytical approximations involved in the extreme relativistic expression (3), it is clear that it would be convenient to have a simple analytic expression for the total cross section, valid over a large range of energies, which reduces in an obvious manner to (3) in the limit of large k. A step in this direction was made in a paper by Hough [7] who gives a corrected expression for the total cross section:

$$\sigma = \bar{\phi}\left(\frac{28}{9}\ln 2k - \frac{218}{27} - \frac{6.45}{k}\right), \tag{4}$$

to be applied at lower energies than those for which (3) may be used. In addition, a number of empirical analytical expressions are given to cover the region $2 \leq k \leq 15$. They are, however, not really very simple, and they do not go smoothly into the high energy expression. Indeed, while the expression (4) is, as far as numerical values are concerned, an improvement over (3) for moderate energies, it is rather deceptive from the analytical standpoint: The corrections to (3) for moderate k are *not* of the form $1/k$. The expression (4) results in fact from an integration of the high energy differential cross section (1) between the limits $\epsilon = 1$ and $\epsilon_1 = k-1$ rather than 0 and k, which leads to (3):

$$\sigma = \frac{4\bar{\phi}}{k^3}\int_0^k \left(\epsilon_1^2 + \epsilon_2^2 + \frac{2}{3}\epsilon_1\epsilon_2\right)\left(\ln\frac{2\epsilon_1\epsilon_2}{k} - \frac{1}{2}\right)d\epsilon_1 = \bar{\phi}\left(\frac{28}{9}\ln 2k - \frac{218}{27}\right), \tag{5}$$

whereas

$$\sigma = \frac{4\bar{\phi}}{k^3}\int_1^{k-1} \left(\epsilon_1^2 + \epsilon_2^2 + \frac{2}{3}\epsilon_1\epsilon_2\right)\left(\ln\frac{2\epsilon_1\epsilon_2}{k} - \frac{1}{2}\right)d\epsilon_1 = \bar{\phi}\left(\frac{28}{9}\ln 2k - \frac{218}{27} + \frac{12-8\ln 2}{k}\right)\left(1 + O\left(\frac{1}{k^2}\right)\right) \tag{6}$$

in which $12-8\ln 2 = 6.45\ldots$

However, the extreme relativistic differential cross section in the integrands here has errors of relative order $1/\epsilon_1^2$ and $1/\epsilon_2^2$, and these may be expected to give contributions of order

$$\frac{1}{k^3}\int_1^{k-1} \frac{\left(\epsilon_1^2 + \epsilon_2^2 + \frac{2}{3}\epsilon_1\epsilon_2\right)}{\epsilon_1^2}\left(\ln\frac{2\epsilon_1\epsilon_2}{k} - \frac{1}{2}\right)d\epsilon_1 = O\left(\frac{\ln k}{k}\right), O\left(\frac{1}{k}\right),$$

i.e., of exactly the same order as the correction calculated by changing the limits of integration from $(0, k)$ to $(1, k-1)$. This is in fact borne out by the expansion given here, in which we see that no terms of the form $1/k$ actually appear in successive terms in the high energy expansion.

In this note we return therefore to the expression for the total cross section without any approximation in the energy, given by Racah, and derive from it two relatively simple and rapidly convergent expansions—one for large k, the other for k near threshold ($k = 2$). The first few terms in each of these expansions are shown to suffice for both analytic and numerical purposes for all k.

The results which we obtain are the following: For k near threshold we derive in fact two series, one in the expansion parameter

$$\eta = \frac{k-2}{k+2}, \tag{7}$$

the other in the somewhat more complicated expansion parameter

$$\rho = \frac{2\eta}{1+\sqrt{1-\eta^2}}. \tag{8}$$

This second series has the advantage of being more rapidly convergent. These expansions are

$$\sigma=\bar{\phi}\,\frac{2\pi}{3}\left(\frac{k-2}{k}\right)^3\left[1+\frac{1}{2}\,\eta+\frac{23}{40}\,\eta^2+\frac{37}{120}\,\eta^3+\frac{61}{192}\,\eta^4+\ldots\right] \tag{9}$$

and

$$\sigma=\bar{\phi}\,\frac{2\pi}{3}\left(\frac{k-2}{k}\right)^3\left[1+\frac{1}{2}\,\rho+\frac{23}{40}\,\rho^2+\frac{11}{60}\,\rho^3+\frac{29}{960}\,\rho^4+\ldots\right]. \tag{10}$$

For large k we derive an expansion in the parameter

$$\mu^2=\left(\frac{2}{k}\right)^2: \tag{11}$$

$$\begin{aligned}\sigma=\bar{\phi}\,\Bigg\{&\frac{28}{9}\ln 2k-\frac{218}{27}\\&+\left(\frac{2}{k}\right)^2\left[6\ln 2k-\frac{7}{2}+\frac{2}{3}\ln^3 2k-\ln^2 2k-\frac{1}{3}\,\pi^2\ln 2k+2\zeta(3)+\frac{\pi^2}{6}\right]\\&-\left(\frac{2}{k}\right)^4\left[\frac{3}{16}\ln 2k+\frac{1}{8}\right]\\&-\left(\frac{2}{k}\right)^6\left[\frac{29}{9\cdot 256}\ln 2k-\frac{77}{27\cdot 512}\right]+\ldots\Bigg\}\end{aligned} \tag{12}$$

where

$$\zeta(3)=\sum_{n=1}^{\infty}\frac{1}{n^3}=1.2020569\ldots$$

The convergence of this high energy expansion is extremely rapid, even for rather low energies. For example, for $k=4$, the fractional error, δ, ($\sigma_{\text{approx}}=\sigma_{\text{exact}}(1+\delta)$) involved in using the terms shown explicitly in (12) is only $+4.4\times10^{-5}$. The fractional errors obtained using the terms shown explicitly in (9) and (10), also for $k=4$, are -1.1×10^{-3} and -1.1×10^{-4}, respectively. For $k>4$, the errors in (12) become smaller and for $k<4$ the errors in (9) and (10) become smaller.

The first term in each of these expansions has been given previously by Racah [8]. Their regions of validity are shown in figure 1, where we give graphs of the ratio of the first term in (10) $\left(\sigma_1^{\text{threshold}}=\bar{\phi}\,\frac{2\pi}{3}\left(\frac{k-2}{k}\right)^3\right)$, and of the first term in (12) $\left(\sigma_1^{\text{E.R.}}=\bar{\phi}\left(\frac{28}{9}\ln 2k-\frac{218}{27}\right)\right)$, to the exact total cross section, σ. It is to be noted from figure 1 that the first term of (10), valid for k near threshold, is more than 10 percent off for $k>1.5$ MeV, and that the first term of (12), valid for k very large, is more than 10 percent off for $k<10$ MeV. In figure 2 we give a graph of the total cross section, σ, in millibarns, as a function of the incident photon energy, k, in MeV. In table 1, values, $(\sigma/\bar{\phi})$, of the total cross section in units of $\bar{\phi}$ are given for photon energies ranging from 1.03 to 1000 MeV.

We proceed now to the derivation of these expansions, our starting point being the exact Born approximation cross section as given by Racah:

$$\begin{aligned}\sigma=\bar{\phi}\,\Bigg\{&\frac{692+468\eta+76\eta^2+108\eta^2}{27(1+\eta)^3}K(\eta)-\frac{692+360\eta+692\eta^2}{27(1+\eta)^3}E(\eta)\\&-4\,\frac{(1-\eta)^2}{(1+\eta)^2}\left[\int_0^{\eta}\frac{K(\xi)}{1-\xi}\,d\xi-4\int_0^{\eta}\frac{d\zeta}{1-\zeta^2}\int_0^{\zeta}\frac{K(\xi)}{1-\xi}\,d\xi\right]\Bigg\}\end{aligned} \tag{13}$$

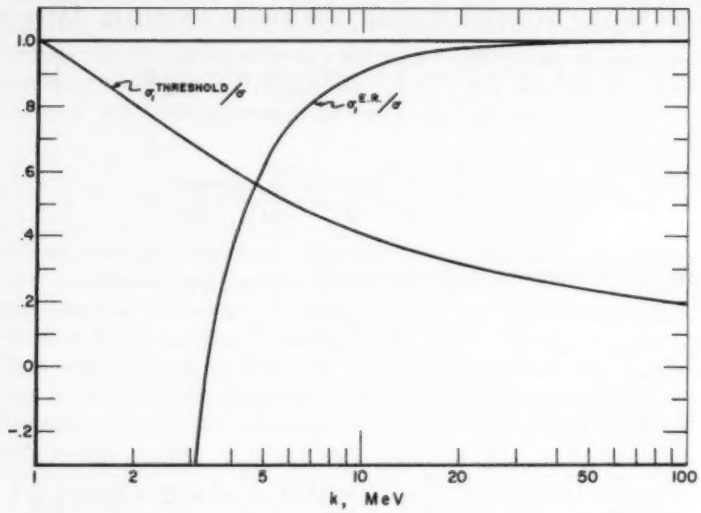


FIGURE 1. *The ratio of the first term in expansion (10)* $\left(\sigma_1^{threshold} = \overline{\phi} \cdot \frac{2\pi}{3}\left(\frac{k-2}{k}\right)^3\right)$, *and of the first term in expansion (12)* $\left(\sigma_1^{E.R.} = \overline{\phi}\left(\frac{28}{9} ln\, 2k - \frac{218}{27}\right)\right)$, *to the exact total cross section,* σ, *as a function of the incident photon energy* k, *in MeV.*

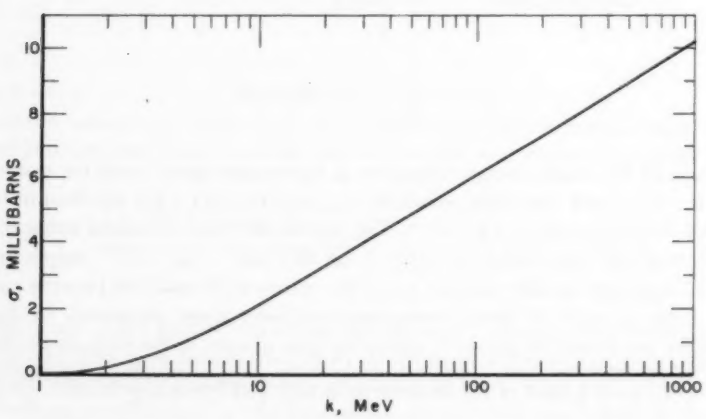


FIGURE 2. *The total pair production cross section,* σ, *in millibarns, as a function of the incident photon energy,* k, *in MeV.*

where $K(\eta)$ and $E(\eta)$ are the complete elliptic integrals of the first and second kind, respectively [9], and are defined by

$$K(\eta) = \int_0^1 \frac{dt}{\sqrt{(1-t^2)(1-\eta^2 t^2)}} \tag{14a}$$

$$= \frac{\pi}{2} F\left(\frac{1}{2}, \frac{1}{2}; 1; \eta^2\right) = \frac{\pi}{2} \sum_{n=0}^{\infty} \frac{\left(\frac{1}{2}\right)_n \left(\frac{1}{2}\right)_n}{n!\, n!} \eta^{2n} \tag{14b}$$

TABLE 1. *The total cross section in units of $\overline{\phi}$ as a function of incident photon energy in MeV*

k (MeV)	$\sigma/\overline{\phi}$	k (MeV)	$\sigma/\overline{\phi}$
1.03	9.788×10^{-7}	10	3.647
1.05	3.994×10^{-5}	15	4.782
1.10	7.607×10^{-4}	20	5.618
1.15	2.978×10^{-3}	30	6.826
1.20	7.134×10^{-3}	40	7.696
1.25	1.342×10^{-2}	50	8.377
1.30	2.189×10^{-2}	60	8.936
1.40	4.507×10^{-2}	80	9.822
1.50	7.577×10^{-2}	100	10.511
1.75	1.777×10^{-1}	150	11.767
2.00	3.030×10^{-1}	200	12.659
2.50	5.836×10^{-1}	300	13.919
3.00	8.716×10^{-1}	400	14.813
4.00	1.416	500	15.507
5.00	1.900	600	16.074
6.00	2.328	800	16.968
8.00	3.052	1000	17.662

$$E(\eta)=\int_0^1 \frac{\sqrt{1-\eta^2t^2}}{\sqrt{1-t^2}}\,dt \tag{15a}$$

$$=\frac{\pi}{2}F\left(-\frac{1}{2},\frac{1}{2};1;\eta^2\right)=\frac{\pi}{2}\sum_{n=0}^{\infty}\frac{\left(-\frac{1}{2}\right)_n\left(\frac{1}{2}\right)_n}{n!\,n!}\eta^{2n} \tag{15b}$$

where $(a)_n=a(a+1)\ldots(a+n-1)$ for $n>0$

and $(a)_0=1$.

Thus for $\eta<1$, we may write out the power series for K and E in (13), integrate term by term, and collect successive powers of η. This straightforward procedure leads to our expansion (9).

Expansion (10) is obtained by using the transformations [9]

$$K(\eta)=(1+\lambda)K(\lambda)=\frac{\pi}{2}(1+\lambda)F\left(\frac{1}{2},\frac{1}{2};1;\lambda^2\right) \tag{16}$$

$$E(\eta)=\frac{2}{1+\lambda}E(\lambda)-(1-\lambda)K(\lambda)=\frac{\pi}{2(1+\lambda)}F\left(-\frac{1}{2},-\frac{1}{2};1;\lambda^2\right) \tag{17}$$

where $$\lambda=\frac{1-\sqrt{1-\eta^2}}{1+\sqrt{1-\eta^2}},\qquad \eta=\frac{2\sqrt{\lambda}}{1+\lambda}. \tag{18}$$

The series for $K(\lambda)$ and $E(\lambda)$ converge faster than those for $K(\eta)$ and $E(\eta)$ since $\lambda<\eta$. Substituting (16), (17) and (18) in (13), we write out the power series for $K(\lambda)$, $E(\lambda)$ and η (a series in $\lambda^{1/2}$), perform the integrations term by term with respect to λ, collect successive powers of $\lambda^{1/2}$ and write the series in terms of the variable $\rho=2\lambda^{1/2}=2\eta/[1+\sqrt{1-\eta^2}]$ since $\rho\to\eta$ as $\eta\to0$. This gives the expansion (10).

In order to obtain the high energy expansion (12), we note that $\eta \sim 1$ for $k \gg 1$. We therefore need expansions of the functions $K(\eta)$ and $E(\eta)$ about $\eta = 1$. To this end we rewrite the transformations (16) and (17) with λ and η interchanged:

$$K(\eta) = \frac{1}{1+\eta} K\left(\frac{2\sqrt{\eta}}{1+\eta}\right) \tag{19}$$

$$E(\eta) = \frac{1+\eta}{2} E\left(\frac{2\sqrt{\eta}}{1+\eta}\right) + \frac{1-\eta}{2} K\left(\frac{2\sqrt{\eta}}{1+\eta}\right). \tag{20}$$

Noting that

$$\frac{2\sqrt{\eta}}{1+\eta} = \sqrt{1-\left(\frac{2}{k}\right)^2} \tag{21}$$

we define

$$\mu = \frac{2}{k}, \qquad \mu' = \sqrt{1-\mu^2} \tag{22}$$

and write (19) and (20) in the form

$$K(\eta) = \frac{k+2}{2k} K(\mu') \tag{23}$$

$$E(\eta) = \frac{k}{k+2} E(\mu') + \frac{2}{k+2} K(\mu'). \tag{24}$$

In (13), the terms preceding the integrals can now be rewritten conveniently in the form

$$\frac{692+468\eta+76\eta^2+108\eta^3}{27(1+\eta)^3} K(\eta) - \frac{692+360\eta+692\eta^2}{27(1+\eta)^3} E(\eta) = \left[\frac{56}{9} + \frac{536}{27k} + \frac{928}{27k^2} + \frac{64}{9k^3}\right] K(\eta)$$

$$-\left[\frac{218}{27} + \frac{512}{27k^2}\right]\left[1+\frac{2}{k}\right] E(\eta) = \frac{2}{27}[42+125\mu^2+6\mu^4] K(\mu') - \frac{2}{27}[109+64\mu^2] E(\mu'). \tag{25}$$

The desired expansions of K and E are

$$K(\mu') = \sum_{n=0}^{\infty} \frac{\left(\frac{1}{2}\right)_n \left(\frac{1}{2}\right)_n}{n!n!} \left[\psi(n+1) - \psi\left(n+\frac{1}{2}\right) - \ln \mu\right] \mu^{2n} \tag{26}$$

$$E(\mu') = 1 + \frac{1}{4} \sum_{n=0}^{\infty} \frac{\left(\frac{1}{2}\right)_n \left(\frac{3}{2}\right)_n}{n!\,(n+1)!} \left[\psi(n+2) + \psi(n+1) - \psi\left(n+\frac{3}{2}\right) - \psi\left(n+\frac{1}{2}\right) - 2\ln\mu\right] \mu^{2n+2} \tag{27}$$

where $\psi(z) = \Gamma'(z)/\Gamma(z)$, and, in particular, [10]

$$\psi(n) = -\gamma + \sum_{l=1}^{n-1} \frac{1}{l}, \qquad n > 0$$

$$\psi\left(n+\frac{1}{2}\right) = -\gamma - 2\ln 2 + 2 \sum_{l=0}^{n-1} \frac{1}{2l+1}, \qquad n > 0$$

$$\psi(0) = -\gamma, \qquad \psi\left(\frac{1}{2}\right) = -\gamma - 2\ln 2 \tag{28}$$

γ = Euler's constant = 0.5772 . . . .

From (28) we may write

$$\psi(n+1)-\psi\left(n+\frac{1}{2}\right)=s_n+2\ln 2$$

where

$$s_n=-2\left[1-\frac{1}{2}+\frac{1}{3}-+\ldots-\frac{1}{2n}\right], \qquad n>0$$

$$s_0=0. \tag{29}$$

Equations (26) and (27) are then written in the form

$$K(\mu')=\sum_{n=0}^{\infty}\frac{\left(\frac{1}{2}\right)_n\left(\frac{1}{2}\right)_n}{n!\,n!}[s_n+\ln 2k]\mu^{2n} \tag{30}$$

$$E(\mu')=1+\frac{1}{4}\sum_{n=0}^{\infty}\frac{\left(\frac{1}{2}\right)_n\left(\frac{3}{2}\right)_n}{n!\,(n+1)!}[s_{n+1}+s_n+2\ln 2k]\mu^{2n+2} \tag{31}$$

Substitution of (30) and (31) in the right hand side of (25) gives the desired high energy expansion of the terms in (13) preceding the integrals. We note that the terms in this expansion are either of the form of a power series in $\mu^2=(2/k)^2$ or $\ln 2k$ times a power series in μ^2.

We next consider the high energy expansion of the integrals in (13). Each of these integrals has the factor

$$\left(\frac{1-\eta}{1+\eta}\right)^2=\left(\frac{2}{k}\right)^2=\mu^2$$

which is precisely our expansion parameter. The first integral is

$$I_1=\int_0^{\eta}\frac{K(\xi)}{1-\xi}\,d\xi. \tag{32}$$

Let

$$\xi=\frac{x-2}{x+2}. \tag{33}$$

from which

$$I_1=\int_2^k\frac{dx}{x+2}K(\xi). \tag{34}$$

Now from (19) we have

$$K(\eta)=\frac{1}{1+\xi}K\left(\frac{2\sqrt{\xi}}{1+\xi}\right)=\frac{x+2}{2x}K\left(\sqrt{1-\left(\frac{2}{x}\right)^2}\right). \tag{35}$$

so that

$$I_1=\frac{1}{2}\int_2^k\frac{dx}{x}K\left(\sqrt{1-\left(\frac{2}{x}\right)^2}\right)=\frac{1}{2}\int_{\frac{2}{k}}^1\frac{dz}{z}K\left(\sqrt{1-z^2}\right), \qquad z=\frac{2}{x}. \tag{36}$$

Since we want an expansion of I_1 for $k \gg 1$, i.e., $2/k \ll 1$, we separate that part of the integrand which becomes singular as $z \to 0$. From (30)

$$K(\sqrt{1-z^2}) - \ln \frac{4}{z} = O(z^2 \ln z) \tag{37}$$

as $z \to 0$. Thus we may write

$$I_1 = \frac{1}{2} \int_{\frac{2}{k}}^{1} \frac{dz}{z} \left[K(\sqrt{1-z^2}) - \ln \frac{4}{z} \right] + \frac{1}{2} \int_{\frac{2}{k}}^{1} \frac{dz}{z} \ln \frac{4}{z}$$

$$= \frac{1}{2} \int_{0}^{1} \frac{dz}{z} \left[K(\sqrt{1-z^2}) - \ln \frac{4}{z} \right] + \frac{1}{4} \ln^2 2k - \ln^2 2 - \frac{1}{2} \int_{0}^{\frac{2}{k}} \frac{dz}{z} \left[K(\sqrt{1-z^2}) - \ln \frac{4}{z} \right]. \tag{38}$$

The evaluation of the definite integral in (38) is given in the appendix. The result is

$$\int_{0}^{1} \frac{dz}{z} \left[K(\sqrt{1-z^2}) - \ln \frac{4}{z} \right] = 2 \ln^2 2 - \frac{1}{12} \pi^2. \tag{39}$$

In the last integral in (38) we substitute (30), with μ replaced by z, $2k$ by $4/z$, and integrate term by term. We then obtain

$$I_1 = \frac{1}{4} \ln^2 2k - \frac{1}{24} \pi^2 - \frac{1}{4} \sum_{n=1}^{\infty} \frac{\left(\frac{1}{2}\right)_n \left(\frac{1}{2}\right)_n}{n!n!n} \left[S_n + \frac{1}{2n} + \ln 2k \right] \left(\frac{2}{k}\right)^{2n}. \tag{40}$$

Finally, we consider the second integral in (13):

$$I_2 = -4 \int_{0}^{\eta} \frac{d\zeta}{1-\zeta^2} \int_{0}^{\zeta} \frac{K(\xi)}{1-\xi} \, d\xi = 2 \int_{0}^{\eta} \left[\ln \left(\frac{1+\xi}{1-\xi} \right) - \ln \left(\frac{1+\eta}{1-\eta} \right) \right] \frac{K(\xi)}{1-\xi} \, d\xi \tag{41}$$

upon integrating by parts. Again we substitute (33) and (35), and obtain

$$I_2 = -2I_1 \ln \frac{k}{2} - \int_{\frac{2}{k}}^{1} \frac{dz}{z} \ln z K(\sqrt{1-z^2}). \tag{42}$$

As with I_1, we write

$$\int_{\frac{2}{k}}^{1} \frac{dz}{z} \ln z K(\sqrt{1-z^2}) = \int_{\frac{2}{k}}^{1} \frac{dz}{z} \ln z \left[K(\sqrt{1-z^2}) - \ln \frac{4}{z} \right] + \int_{\frac{2}{k}}^{1} \frac{dz}{z} \ln z \ln \frac{4}{z}$$

$$= \int_{0}^{1} \frac{dz}{z} \ln z \left[K(\sqrt{1-z^2}) - \ln \frac{4}{z} \right] + \frac{1}{3} \ln^3 \frac{2}{k} - \ln 2 \ln^2 \frac{2}{k} - \int_{0}^{\frac{2}{k}} \frac{dz}{z} \ln z \left[K(\sqrt{1-z^2}) - \ln \frac{4}{z} \right]. \tag{43}$$

The evaluation of the first integral here is also given in the appendix. The result is

$$\int_{0}^{1} \frac{dz}{z} \ln z \left[K(\sqrt{1-z^2}) - \ln \frac{4}{z} \right] = \frac{4}{3} \ln^3 2 - \frac{1}{6} \pi^2 \ln 2 - \frac{1}{2} \zeta(3). \tag{44}$$

In the last integral in (43) in we again substitute (30) and integrate term by term. Since these integrals appear in (13) only in the form of the sum I_1+I_2, we give this result:

$$I_1+I_2=-\frac{1}{6}\ln^3 2k+\frac{1}{4}\ln^2 2k+\frac{1}{12}\pi^2\ln 2k-\frac{1}{24}\pi^2-\frac{1}{2}\zeta(3)$$

$$-\frac{1}{4}\sum_{n=1}^{\infty}\frac{\left(\frac{1}{2}\right)_n\left(\frac{1}{2}\right)_n(n+1)}{n!n!n^2}\left[\ln 2k+s_n+\frac{n+2}{2n(n+1)}\right]\left(\frac{2}{k}\right)^{2n} \tag{45}$$

Appendix

We evaluate here the definite integrals appearing in (38) and (43):

$$J_1=\int_0^1\frac{dz}{z}\left[K)\sqrt{1-z^2}\right)-\ln\frac{4}{z}\Big] \tag{A.1}$$

$$J_2=\int_0^1\frac{dz}{z}\ln z\left[K(\sqrt{1-z^2})-\ln\frac{4}{z}\right]. \tag{A.2}$$

We define

$$J(\alpha)=\int_0^1\left[K(\sqrt{1-z^2})-\ln\frac{4}{z}\right]z^{-1+2\alpha}dz \tag{A.3}$$

with $\alpha\geq 0$, so that

$$J_1=J(0) \tag{A.4}$$

$$J_2=\frac{1}{2}J'(0). \tag{A.5}$$

Substituting $t=1-z^2$ in (A.3) and using (14b), we have

$$J(\alpha)=\frac{\pi}{4}\int_0^1(1-t)^{-1+\alpha}F\left(\frac{1}{2},\frac{1}{2};1;t\right)dt+\frac{1}{4}\int_0^1(1-t)^{-1+\alpha}\ln\frac{1-t}{16}dt. \tag{A.6}$$

Here

$$\int_0^1(1-t)^{-1+\alpha}dt=\frac{1}{\alpha},$$

$$\int_0^1(1-t)^{-1+\alpha}\ln(1-t)dt=\frac{d}{d\alpha}\int_0^1(1-t)^{-1+\alpha}dt=-\frac{1}{\alpha^2} \tag{A.7}$$

and [11]

$$\int_0^1(1-t)^{-1+\alpha}F\left(\frac{1}{2},\frac{1}{2};1;t\right)dt=\frac{\Gamma(\alpha)}{\Gamma(\alpha+1)}F\left(\frac{1}{2},\frac{1}{2};1+\alpha;1\right)=\left[\frac{\Gamma(\alpha)}{\Gamma\left(\alpha+\frac{1}{2}\right)}\right]^2.$$

Thus

$$J(\alpha)=\frac{\Gamma^2\left(\frac{1}{2}\right)\Gamma^2(\alpha+1)-\Gamma^2\left(\alpha+\frac{1}{2}\right)-4\alpha\Gamma^2\left(\alpha+\frac{1}{2}\right)\ln 2}{4\alpha^2\Gamma^2\left(\alpha+\frac{1}{2}\right)}. \tag{A.8}$$

We then expand this expression in a power series in α, keeping, in the final result, terms linear in α. We note

$$\Gamma'(z)=\psi(z)\Gamma(z)$$

$$\Gamma''(z)=\psi'(z)\Gamma(z)+\psi^2(z)\Gamma(z) \tag{A.9}$$

and the following values for specific values of z: [10]

$$\Gamma(1)=1, \qquad \Gamma\left(\frac{1}{2}\right)=\pi^{1/2}$$

$$\psi(1)=-\gamma, \qquad \psi\left(\frac{1}{2}\right)=-\gamma-2\ln 2$$

$$\psi'(1)=\frac{\pi^2}{6}, \qquad \psi'\left(\frac{1}{2}\right)=\frac{\pi^2}{2}$$

$$\psi''(1)=-2\zeta(3), \qquad \psi''\left(\frac{1}{2}\right)=-14\zeta(3)$$

$$\zeta(3)=\sum_{n=1}^{\infty}\frac{1}{n^3}=1.2020569\ldots \tag{A.10}$$

We find

$$J(\alpha)=2\ln^2 2-\frac{1}{12}\pi^2+\alpha\left[\frac{8}{3}\ln^3 2-\frac{1}{3}\pi^2\ln 2-\zeta(3)\right]+O(\alpha^2) \tag{A.11}$$

from which J_1 and J_2 follow from (A.4) and (A.5).

We would like to express our thanks to J. H. Hubbell for performing the computer calculations involved in the preparation of figures 1 and 2 and table 1.

References

[1] W. Heitler and F. Sauter, Nature **132**, 892 (1933).
[2] H. Bethe and W. Heitler, Proc. Roy. Soc. London, Ser. A **146**, 83 (1934).
[3] W. Heitler, The Quantum Theory of Radiation, third edition, pp. 256–267. (Oxford University Press, London, 1954).
[4] Giulio Racah, Nuovo Cimento **11**, 477 (1934) and **13**, 66 (1936). In the latter article, note p. 69, Eqs (10), (11) and the footnote on p. 69, where a typographical error in Eq (10) of the former paper is corrected.
[5] Ref. 3, p. 258, Eq (8).
[6] Ref. 3, p. 258, Eq (9).
[7] P. V. C. Hough, Phys. Rev. **73**, 266 (1948).
[8] In Ref. 4, Nuovo Cimento **11**, note p. 480, Eq (12).
[9] W. Gröbner and N. Hofreiter, Integroltafel, Vol. II (Springer-Verlag, Vienna, 3rd ed. 1961). Note pp. 39, 40.
[10] W. Magnus, F. Oberhettinger, and R. P. Soni, Formulas and Theorems for the Special Functions of Mathematical Physics (Springer-Verlag, New York, Inc., 1966). Note, p. 15.
[11] Ref. 9, pp. 40 and 55.

(Paper 72B1–261)

JOURNAL OF RESEARCH of the National Bureau of Standards—B. Mathematical Sciences
Vol. 72B, No. 1, January–March 1968

Publications of the National Bureau of Standards*

Selected Abstracts

A modified Monte-Carlo quadrature. II, S. Haber, *Math. Compt.* **21,** *No. 99, 388–397 (July 1967).*
A modification of Simple Monte-Carlo quadrature is proposed, which uses very simple forms of stratified sampling and of the "method of antithetic variates." The new procedure is fully automatic—requiring no preliminary analysis of the integrand—and converges somewhat faster than Simple Monte-Carlo. Results of experimental calculations are presented.

Key Words: Mathematics, analysis, numerical analysis, integration, numerical integration, quadrature, Monte-Carlo, multiple integration.

Note on partitions modulo 5, M. Newman, *Math. Compt.* **21,** *No. 99, 481–482 (July 1967).*
It is shown that the density of the integers n such that $p(n)$ is divisible by 5, is strictly greater than $\frac{1}{5}$.

Key Words: Partitions, density, Ramanujan congruences.

Proof of a permanental inequality, R. A. Brualdi and M. Newman, *Quart. J. Math.* **17,** *No. 67, 234–238 (Sept. 1966).*
The principal result of this note is that if A is a non-negative row-stochastic matrix then per $(I-A) \geq 0$ where per (A) denotes the permanent of A. The case of equality is discussed.

Key Words: Inequalities, permanental, symmetric, matrices.

Other NBS Publications

J. Res. NBS 72A, (Phys. and Chem.), No. 1, (Jan.–Feb. 1968), $1.00
Reactions of uranium with the platinide elements. I. The uranium-ruthenium system. J. J. Park.
Reactions of uranium and the platinide elements. II. The uranium-rhodium system. J. J. Park.
Reactions of uranium and the platinide elements. III. The uranium-iridium system. J. J. Park and L. R. Mullen.
Phase relations between palladium oxide and the rare earth sesquioxides in air. C. L. McDaniel and S. J. Schneider.
Preparation and purification of some oxidation products of perylene. A. J. Fatiadi.
Electron spin resonance spectra of polymer radicals in aqueous solution. R. E. Florin, F. Sicilio, and L. A. Wall.
A mass spectrometric study of the BeO–BeF_2 system at high temperatures. J. Efimenko.
Laser induced Raman spectra of some tungstates and molybdates. R. K. Khanna, W. S. Brower, B. R. Guscott, and E. R. Lippincott.
Valance-only correlation in LiH and BeH^+. W. A. Sanders and M. Krauss.
Thermalization by elastic collisions: positronium in a rare gas moderator. W. C. Sauder.
Density fluctuations in fluids having an internal degree of freedom. R. D. Mountain.

Analytical Mass Spectrometry Section: Summary of activities July 1966 to June 1967, Ed. W. R. Shields, Tech. Note 426 (Sept. 15, 1967), 40 cents.
Comparison of incompressible flow and isothermal compressible flow formulae, J. Hord, Tech. Note 356 (Aug. 17, 1967), 25 cents.
Correlations for predicting leakage through closed valves, J. Hord, Tech. Note 355 (Aug. 1, 1967), 20 cents.
Designs for surveillance of the volt maintained by a small group of saturated standard cells, W. G. Eicke and J. M. Cameron, Tech. Note 430 (Oct. 9, 1967), 20 cents.
Electrochemical Analysis Section: Summary of activities July 1966 to June 1967, Ed. R. G. Bates, Tech. Note 423 (Oct. 1967), 50 cents.
Field burnout tests of apartment dwelling units, D. Gross, Bldg. Sci. Series 10 (Sept. 29, 1967), 25 cents.
"Life cycling" test on several strain gage pressure transducers, P. S. Lederer, Tech. Note 434 (Oct. 1967), 20 cents.
Loading factors and FDM-FM system performance calculations, E. F. Florman, Tech. Note 100–A (Sept. 1967), 20 cents. Supplement to Appendix C of Tech. Note 100.
Microchemical Analysis Section: Summary of activities July 1966 to June 1967, Ed. J. K. Taylor, Tech. Note 425 (Oct. 1967), 50 cents.
Organic Chemistry; Air pollution studies characterization of chemical structures; synthesis of research materials; novel research materials; isotopic methods for analysis of carbohydrates; occurrence, preparation, and properties of naturally occurring monosaccharides (including 6-deoxy sugars); standard reference materials (organic) July 1966 through June 1967, Ed. R. Schaffer, Tech. Note 427 (Oct. 1967), 45 cents.
Photonuclear data index, January 1965 through April 1967, Misc. Publ. 277, Supplement 1 (Oct. 1967), 45 cents.
Radiometric methods for measuring laser output, D. A. McSparron, C. A. Douglas, and H. L. Badger, Tech. Note 418 (Nov. 1967), 15 cents.
Realistic uncertainties and the mass measurement process. An illustrated review, P. E. Pontius and J. M. Cameron, Mono. 103 (Aug. 15, 1967), 20 cents.
Second breakdown in semiconductor devices—A bibliography, H. A. Schafft, Tech. Note 431 (Oct. 1967), 30 cents.
Selected values of electric dipole moments for molecules in the gas phase, R. D. Nelson, Jr., D. R. Lide, Jr., and A. A. Maryott, NSRDS–NBS10 (Sept. 1, 1967), 40 cents. (Supersedes the data on dipole moments included in NBS Circ. 537.)
Standard Reference Materials: Catalog and price list of standard materials issued by the National Bureau of Standards, Misc. Publ. 260, 1967 edition (Sept. 15, 1967), 45 cents. (Supersedes NBS Misc. Publ. 260, 1965 edition.)
Standard x-ray diffraction powder patterns, H. E. Swanson, H. F. McMurdie, M. C. Morris, and E. H. Evans, Mono. 25, Sect. 5 (Aug. 31, 1967), 55 cents.
Tables of molecular vibrational frequencies Part 2, T. Shimanouchi, NSRDS–NBS 11 (Oct. 1967), 30 cents.
1967 Technical Highlights of the National Bureau of Standards, Annual Report, Fiscal Year 1967, Misc. Publ. 293 (Nov. 1967), 55 cents.
X-ray wavelength conversion tables and graphs for qualitative electron probe microanalysis, K. F. J. Heinrich and M. A. M. Giles, Tech. Note 406 (Sept. 25, 1967), 70 cents.
X-ray wavelengths and x-ray atomic energy levels, J. A. Bearden, NSRDS–NBS 14 (Sept. 25, 1967), 40 cents.
A method of producing sturdy specimens of pressed powders for use in x-ray spectrochemical analysis, B. L. Bean, Appl. Spectry. **20,** No. 3, 191–193 (May-June 1966).
Aromatic fluorocarbon polymers, W. J. Pummer and J. M. Antonucci (Proc. 152nd American Chemical Society Meeting, New York, N.Y., Sept. 13, 1966), Polymer Preprint **7,** No. 2, *1071–1076* (Sept. 1966).

Calculation of currents of local galvanic cells, J. A. Simmons, S. R. Coriell, and F. Ogburn, J. Electrochem. Soc. **114,** No. 8, 782–787 Aug. 1967).

Conformation of polystyrene adsorbed on liquid mercury, R. R. Stromberg and L. E. Smith, J. Phys. Chem. **71,** No. 8, 2470–2474 (July 1967).

Crystallization of natural rubber, N. Bekkedahl, Rubber Chem. Technol. **40,** No. 3, xxv-xlvii (June 1967).

Determination of bound styrene in insoluble emulsion polymerized styrene-butadiene copolymers, M. A. Post, J. Appl. Chem. **17,** 203–208 (July 1967).

Effects of impurities on the production of oxygen atoms by a microwave discharge, R. L. Brown, J. Phys. Chem. **71,** No. 8, 2492–2495 (1967).

Electrical conductivity of high purity copper, J. J. Gniewek, J. C. Moulder, and R. H. Kropschot, Proc. LT–10 Conf., Moscow, USSR, Aug. 31-Sept. 9, 1966.

Epitaxial growth of iron on tungsten field emission points, A. J. Melmed, Surface Sci. **7,** No. 3, 478–481 (July 1967).

Growth of large sodium chloride crystals from solution for color center studies, P. M. Gruzensky, J. Chem. Phys. **43,** No. 11, 3807 (Dec. 1, 1965).

Helium field-ion microscopy of hexagonal close-packed metals, A. J. Melmed (Proc. Symp. The Structure of Surfaces, Durham, N.C., Nov. 1966), Surface Sci. **8,** No. 12, 191–205 (July–Aug. 1967).

High pressure adsorption isotherms of neon, hydrogen, and helium at 76 °K, A. J. Kidnay and M. J. Hiza (Proc. 1966 Conf., Boulder, Colo., June 13–15, 1966), Book, Advances in Cryogenic Engineering **12,** 730–740 (Plenum Press Inc., New York, N.Y., 1967).

History of the National Standard of electromotive force, W. J. Hamer, (Proc. 22nd ISA Conf. and Exhibit, Chicago, Ill., Sept. 11–14, 1967), ISA Preprint No. M2–1–MESTIND–67, pp. 1–10 (1967).

Indentation hardness of the fingernail, S. B. Newman and R. W. Young, J. Invest. Dermatol. **49,** No. 1, 103–105 (Mar. 17, 1967).

Insertion of methylene into alkanes, M. L. Halberstadt and J. R. McNesby, J. Am. Chem. Soc. **89,** No. 14, 3417–3420 (1967).

Liquid-vapor equilibrium in the system helium-methane, C. K. Heck and M. J. Hiza, AIChE. J. **13,** No. 3, 593–599 (May 1967).

Polymerization of fluoroolefins and related monomers, L. A. Wall (Proc. 152nd American Chemical Society Meeting, New York, N.Y., Sept. 13, 1966), Polymer Preprint **7,** No. 2, 1112–1115 (Sept. 1966).

The system Y_2O_3-V_2O_5, E. M. Levin, J. Am. Ceram. Soc. **50,** No. 7, 381–382 (July 1967).

The thermal decomposition of poly-3,3,3,-tri-fluoropropene made at high pressure, S. Straus and D. W. Brown (Proc. 152nd American Chemical Society Meeting, New York, N.Y., Sept. 13, 1966), Polymer Preprint **7,** No. 2, 1128–1132 (Sept. 1966).

The unperturbed dimension temperature coefficients of some fluorine-containing polymers, H. Yu (Proc. 152nd American Chemical Society Meeting, New York, N.Y., Sept. 13, 1966), Polymer Preprint **7,** No. 2, 1143–1145 (Sept. 1966).

A computer simulation model of railroad freight transportation systems, W. P. Allman, Intern. Railway Cong. Assoc. Mo. Bull. Cybernetics and Electronics **4,** No. 2, 45–57 (Feb. 1967).

A precision noise power comparator, M. G. Arthur, C. M. Allred, and M. K. Cannon, IEEE Trans. Instr. Meas. IM–4, 301–305 (Dec. 1964).

Electronic computer applications in urban transportation planning, R. E. Schofer and F. F. Goodyear (Proc. 22nd Natl. Conf. Association for Computing Machinery, Washington, D.C., Aug. 29–31, 1967), A. C. M. Publ. P–67, pp. 247–253 (Thompson Book Co., Washington, D.C., July 1967).

Microprinting fills the bill, B. M. Fry, Business Graphics, pp. 21–25 (Jan. 1967).

Microwave standards and measurements in the USA, R. W. Beatty (Proc. XV General Assembly of URSI, Munich, Germany, Sept. 5–15, 1966), Book, Progress in Radio Science 1963–1966, Part 1, pp. 194–260 (International Scientific Radio Union, Munich, Germany, 1966).

Proposed recommended practice for description and selection of conditions for photographing specimens, C. S. McCamy, Photo. Sci. Eng. **10,** No. 4, 185–191 (July–Aug. 1966).

Protection circuit insulated for high voltage, E. Niesen, Rev. Sci. Instr. **38,** No. 5, 689 (May 1967).

Remarks for XV URSI General Assembly session on progress at $f \leq 1$ GHz, M. C. Selby (Proc. XV General Assembly of URSI, Munich, Germany, Sept. 5–15, 1966), Book, Progress in Radio Science 1963–1966, Part 1, pp. 157–162 (International Scientific Radio Union, Munich, Germany, Sept. 1966).

Scanning the issue, R. W. Beatty and B. O. Weinschel, Proc. IEEE **55,** No. 6, 737–740 (June 1967).

Size and power requirements of 4.2 °K refrigerators, T. R. Strowbridge and D. E. Chelton (Proc. 1966 Conf., Cryogenic Engineering, Boulder, Colo., June 13–15, 1966).

Book, Advances in Cryogenic Engineering **12,** 576–584 (Plenum Press, Inc., New York, N.Y., 1967).

Slush hydrogen characteristics, D. B. Mann, C. F. Sindt, P. R. Ludtke, and D. B. Chelton, Proc. Conf. Long-Term Cryo-Propellant Storage in Space, National Aeronautics and Space Administration, Huntsville, Ala., Oct. 12–13, 1966.

The role of NBS in motor vehicle safety research, P. J. Brown, Proc. Regional Meeting Society Automotive Engineers, Gaithersburg, Md., Apr. 18, 1967, SAE 670204, p. 3 (June 1967).

Aggregation in matrix models of resource flows. II. Boolean relation matrix methods, D. R. Rosenblatt, Am. Stat. **21,** No. 3, 32–37 (June 1967).

Current distribution and impedance of lossless conductor systems, R. L. Brooke and J. E. Cruz, IEEE Trans. Microwave Theory Tech. **MTT–15,** No. 6, 358–364 (June 1967).

Scheduling a vehicle between an origin and a destination to maximize traveler satisfaction, D. Young (Proc. 22nd Natl. Conf. Association for Computing Machinery, Washington, D.C., Aug. 29–31, 1967), A. C. M. Publ. P–67, pp. 233–245 (Thompson Book Co., Washington, D.C., July 1967).

The spheroidal method in satellite astronomy, J. P. Vinti, Book, Space Mathematics 5, Part 1, 119–129 (American Mathematical Society, Providence, R.I., 1966).

A systems concept of electromagnetic measurements in the U.S.A., G. E. Schafer, Proc. IEEE **55,** No. 6, 775–778 (June 1967).

Linear measurements, T. R. Young, Book, Handbook of Industrial Metrology, Chapt. 3, pp. 55–81 (Prentice-Hall, Inc., Englewood Cliffs, N.J., 1967).

Liquid hydrogen engineering instrumentation, T. M. Flynn (Proc. Intern. Inst. Refrigeration, June 9–11, 1965), Book, Liquid Hydrogen, pp. 295–338 (Paris, France, 1965).

Progress in the distribution of standard time and frequency, 1963 through 1965, J. M. Richardson (Proc. XV General Assembly of URSI, Munich, Germany, Sept. 5–15, 1966), Book, Progress in Radio Science 1963–1966, Part 1, pp. 40–62 (International Scientific Radio Union, Munich, Germany, 1966).

Progress in the U.S. on electromagnetic standards and measurements at 30 kHz to 1 GHz, 1963 through 1965, M. C. Selby, IEEE Trans. Instr. Meas. **IM–16,** No. 2, 172–178 (June 1967).

The conference on precision electromagnetic measurements, H. M. Altschuler, Proc. IEEE **55,** No. 6, 782 (June 1967).

The nature of measurement, A. G. McNish, Book, Handbook of Industrial Metrology, ch. 1, pp. 2–12 (Prentice-Hall, Inc., Englewood Cliffs, N.Y., 1967).

The role of the NBS Radio Standards Laboratory, H. M. Altschuler, Proc. IEEE **55,** No. 6, 778–781 (June 1967).

U.S.A. National Committee Report, Fifteenth URSI General Assembly, Munich, September 1966: Commission 1, Radio Measurement Methods and Standards, Progress in Radio Measurement Methods and Standards, J. M. Richardson, Editor, Radio Science **1,** No. 11, 1333–1342 (Nov. 1966).

Cyclotron harmonic emission from the abnormal negative glow plasma, K.-B. Persson, D. A. Uhlenbrock, and E. G. Johnson, Bull. Am. Phys. Soc. **12,** Series II, No. 5, 756 (May 1967).

Dissociative ionization of H_2 and D_2, L. J. Kieffer and G. H. Dunn, Phys. Rev. **158,** No. 1, 61–65 (June 5, 1967).

F^{19} relaxation in AFM $KMnF_3$, P. T. Parrish, A. C. Daniel, and R. J. Mahler, Bull. Am. Phys. Soc. **12,** Series II, No. 3, 284 (Mar. 1967).

Interpretation of de Grinberg's experiments on lateral surface fringes in sodium chloride, H. P. Utech, Phys. Stat. Solidi **20,** K41–K43 (1967).

Laser measurements of long distances, P. L. Bender, Proc. IEEE **55,** No. 6, 1039–1045 (June 1967).

Low temperature (295–4 K) mechanical properties of selected copper alloys, R. P. Reed and R. Mikesell, J. Materials **2,** No. 2, 370–392 (June 1967).

Metrology, essential of space age, A. G. McNish, George Washington University Mag. **1,** No. 4, 10–14 (1965).

Non-linear diffusion with recombination in electron beam excited plasma, E. R. Mosburg, Jr. and M. S. Lojko, Phys. Fluid Res. Notes **9,** No. 4, 824–826 (Apr. 1966).

Optical properties of germanium in the far ultraviolet, L. Marton and J. Toots, Phys. Rev. **160,** No. 3, 602–606 (Aug. 15, 1967).

Positive and negative self-surface ionization of tungsten and rhenium, M. D. Scheer and J. Fine, J. Chem. Phys. **46,** No. 10, 3998–4003 (May 15, 1967).

Properties of liquid hydrogen, R. J. Corruccini (Proc. Intern. Inst. Refrigeration, June 9–11, 1965), Book, Liquid Hydrogen, pp. 65–106 (Paris, France, 1965).

Reply by A. G. McNish, Phys. Today **19,** No. 4, 15–16 (Apr. 1966).

Reply to "comments on Reed letter, by H. M. Otte," R. P. Reed, Acta. Met. **15,** No. 6, 1082–1083 (June 1967).

Surface self-diffusion of nickel and platinum, A. J. Melmed, J. Appl. Phys. **38,** No. 4, 1885–1892 (Mar. 1967).

The aurora, A. G. McNish, Proc. NATO Advanced Study Institute, Bad Homburg, Germany, July 22–Aug. 2, 1963, Ed. D. S. Bleil, pp. 77–93 (Plenum Press Inc., New York, N.Y., 1964).

U.S. Department of Commerce and the flammability of clothing fabric, A. F. Robertson, Bull. N.Y. Acad. Med. Second Series **43,** No. 8, 706–710 (Aug. 1967).

Brief report of the XV URSI General Assembly, Commission I, on the status of international intercomparisons of high frequency and microwave electrical quantities, M. C. Selby (Proc. XV General Assembly of URSI, Munich, Germany, Sept. 5–15, 1966), Book, Progress in Radio Science 1963–1966, Part 1, pp. 113–116 (International Scientific Radio Union, Munich, Germany, Sept. 1966).

Perturbation theorems for waveguide junctions, with applications, D. M. Kerns and W. T. Grandy, Jr., IEEE Trans. Microwave Theory Tech. **MTT-14,** No. 2, 85–92 (Feb. 1966).

Progress in measurement of electromagnetic properties of material, 1963 to mid-1966, H. E. Bussey (Proc. XV General Assembly of URSI, Munich, Germany, Sept. 5–15, 1966), Book, Progress in Radio Science 1963–1966, Part 1, pp. 265–289 (International Scientific Radio Union, Munich, Germany, 1966).

A novel, facile preparation of 1,1′-bipyrene, A. J. Fatiadi, J. Org. Chem. **32,** 2903–2904 (Sept. 1967).

Comment on "paramagnetic resonance of alkyl nitroxides," R. E. Florin, J. Chem. Phys. **47,** No. 1, 345–346 (July 1, 1967).

Development of an adhesive restorative material, R. L. Bowen (Proc. 2d Workshop, Adhesive Restorative Dental Materials, University of Virginia, Charlottesville, Va., Dec. 8–9, 1965), Book, Adhesive Restorative Dental Materials, No. 2, ch. 4, p. 225 (U.S. Public Health Service Publ. 1494, Supt. Docs. Government Printing Office, Washington, D.C. 20402, $1.00, 1966).

Excited species and their contribution to NO (β, γ) fluorescence in the photodissociation of N_2O, H. Okabe, J. Chem. Phys. **47,** No. 1, 101–109 (July 1, 1967).

Identification of dyes in paper by extraction and chromatographic analysis, M. R. Wallace, L. T. Milliken, and S. D. Toner, TAPPI **50,** No. 9, 121A–124A (Sept. 1967).

Interpretation of cyclotron resonance line shapes in slightly ionized gases, F. C. Fehsenfeld, L. R. Megill, and L. K. Dropplemann, J. Chem. Phys. **43,** No. 10, 3618–3624 (Nov. 1965).

Matrix-isolation study of the reaction of carbon atoms with chlorine. The electronic and vibrational spectra of the free radical CCl_2, D. E. Milligan and M. E. Jacox, J. Chem. Phys. **47,** No. 2, 703–707 (July 15, 1967).

Measurement of density and specific gravity, J. K. Taylor, Book, Treatise on Analytical Chemistry, Ed. I. M. Kolthoff, P. J. Elving, and E. B. Sandell, Part 1, Theory and Practice, 7, ch. 81, 4561–4610 (Interscience Publ., New York, N.Y., 1967).

Modification of the fluoride activity electrode for microchemical analysis, R. A. Durst and J. K. Taylor, Anal. Chem. **39,** No. 12, 1483–1485 (Oct. 1967).

Modified linear null-point potentiometry, R. A. Durst and J. K. Taylor, J. Chem. Educ. **39,** No. 12, 1374–1379 (Oct. 1967).

On the structure of pyrazole, A. D. Mighell and C. W. Reimann, J. Phys. Chem. **71,** No. 7, 2375–2376 (June 1967).

Optical and magnetic measurements on single crystals of copper(II)-doped tris(phenanthroline)zinc(II) nitrate dihydrate, G. F. Kokoszka, C. W. Reimann, H. C. Allen, Jr., and G. Gordon, Inorg. Chem. **6,** No. 9, 1657–1661 (1967).

Polymerization and pyrolysis of poly-1,2-dihydronaphthalene, L. A. Wall, L. J. Fetters, and S. Straus, Polymer Letters **5,** No. 8, 721–733 (Aug. 1967).

Spectroscopic study of the vacuum-ultraviolet photolysis of matrix-isolated HCN and halogen cyanides. Infrared spectra of the species CN and XNC, D. E. Milligan and M. E. Jacox, J. Chem. Phys. **47,** No. 1, 278–285 (July 1, 1967).

The crystal and molecular structure of tetrakispyrazole-nickel chloride, $Ni(C_6H_4N_2)_4Cl_2$, C. W. Reimann, A. D. Mighell, and F. A. Mauer, Acta Cryst. **23,** Part 1, 135–141 (July 1967).

The determination of bound styrene in insoluble emulsion polymerized styrene-butadiene copolymers, M. A. Post, J. Appl. Chem. **17,** 203–208 (July 1967).

Vacuum-ultraviolet photolysis of acetylene in inert matrices. Spectroscopic study of the species C_2, D. E. Milligan, M. E. Jacox, and L. Abouaf-Marguin, J. Chem. Phys. **46,** No. 12, 4562–4570 (June 15, 1967).

Dead weight piston gauge for pressures to 26 kilobars, D. P. Johnson and P. L. M. Heydemann, Rev. Sci. Instr. **38,** No. 9, 1294–1300 (Sept. 1967).

Lou Costrell of NBS speaks out on the revolution in instrument packaging, L. Costrell, EEE **15,** No. 8, 78–84 (Aug. 1967).

C. S. Pierce on benefit-cost analysis of scientific activity, W. E. Cushen, Operations Res. **15,** No. 4, p. 641 (July–Aug. 1967).

Editor and translater, H. J. Oser, Book, Functional Analysis and Numerical Mathematics, by L. Collatz (Academic Press Inc., New York, N.Y., 1966).

Localized-induction concept on a curved vortex and motion of an elliptic vortex ring, R. J. Arms and F. R. Hama, Phys. Fluids **8,** No. 4, 553–559 (Apr. 1965).

Robust estimation of location, E. L. Crow and M. M. Siddiqui, J. Am. Stat. Assoc. **62,** No. 318, 353–389 (June 1967).

Coping with multiple reflections in precise measurement of the speed of light with a microwave Michelson interferometer, D. M. Kerns (Proc. URSI Symp. Electromagnetic Wave Theory, Delft, The Netherlands, September 1965), Book, Electromagnetic Wave Theory, pp. 245–249 (Pergamon Press Inc., New York, N.Y., 1967).

Low-frequency electrical calibrations at the National Bureau of Standards, F. L. Hermach (Proc. 22nd Annual ISA Conf. and Exhibit, Chicago, Ill., Sept. 11–14, 1967), ISA Preprint M5–1–MESTIND–67 (May 1967).

Measurement standards, A. G. McNish, IEEE Student J. **4,** No. 2, 24–31 (Mar. 1966).

The functions of Commission I of the International Scientific Radio Union, J. M. Richardson, Proc. IEEE **55,** No. 6, 743–745 (June 1967).

A note on the evaluation of interference photographs, J. R. Meyer-Arendt, Acta Histochem. **22,** 58–61 (1965).

A simple, inexpensive wavefront shearing interferometer, J. B. Saunders, Appl. Opt. **6,** No. 9, 1581–1583 (Sept. 1967).

Angular scattering law for the moon at 6 meter wavelength, W. K. Klemperer, J. Geophys. Res. Letter **70,** No. 15, 3798–3800 (Aug. 1965).

Application of the Fock expansion to doubly excited states of the helium atom, J. H. Macek, Phys. Rev. **160,** No. 1, 170–174 (Aug. 5, 1967).

Characteristic energy losses of 8 KeV electrons in liquid In-Al and In-Bi alloys, C. J. Powell, Advan. Phys. **16,** 203 (1967).

Characteristics of a slotted-sphere antenna immersed in a compressible plasma, J. R. Wait (Proc. Conf. Microwave Behaviour of Ferrimagnetics and Plasmas), Conf. Publ. No. 13, pp. 1–4 (Inst. Electrical Engineers, London, England, 1965).

Cross section for Na ($^2P_{1/2}$, $^2P_{3/2}$) intramultiplet transactions induced by collisions with the hydrogen atoms, R. N. Zare and P. L. Bender, Proc. Am. Phys. Soc. Meeting, Los Angeles, Calif., 10, 1183 (American Physical Society, New York, N.Y., 1965).

Definitions of v, i, Z, Y, a, b, Γ, and S, D. M. Kerns, Proc. IEEE **55,** No. 6, 892–900 (June 1967).

Equations of motion in nonequilibrium statistical mechanics. II. Energy transport, B. Robertson, Phys. Rev. **160,** No. 1, 175–183 (Aug. 5, 1967).

Equivalence between two formalisms of plasma fluctuations, J. Weinstock, Phys. Fluids **9,** No. 3, 621–622 (Mar. 1966).

Experimental determination of transition probabilities and Stark widths of S I and S II lines, J. M. Bridges and W. L. Wiese, Phys. Rev. 159, No. 1, 31–38 (July 5, 1967).

Hall mobility in $SrTiO_3$, H. P. R. Frederikse and W. R. Hosler, Phys. Rev. **161,** No. 3, 822–827 (Sept. 15, 1967).

Ionosphere, T. E. VanZandt, Encyclopedia of Physics, Ed. R. M. Besancon, pp. 348–349 (Reinhold Publ. Co., New York, N.Y., 1966).

Lifetimes of some 4p levels in argon I, J. Z. Klose, J. Opt. Soc. Am. **57**, No. 10, 1242–1244 (Oct. 1967).

Measurements of Stark profiles of C II and Ca II lines, J. R. Roberts and K. L. Eckerle, Phys. Rev. **159**, No. 1, 104–107 (July 5, 1967).

Mechanistic aspects of hearing, E. L. R. Corliss, J. Acoust. Soc. Am. **41**, No. 6, 1500–1516 (June 1967).

Nature of ionic deformations in crystals; application to an analysis of the magnetic properties of the alkalihalide and alkaline-earth oxide crystals, A. R. Ruffa, Phys. Rev. **159**, No. 3, 742–754 (July 15, 1967).

Nuclear magnetic acoustic resonance in $KTaO_3$, R. W. Mebs, L. H. Bennett, and J. R. Leibowitz, Physics Letters **24A**, No. 12, 665–666 (June 5, 1967).

On the explanation of the so-called CN laser, D. R. Lide, Jr. and A. G. Maki, Appl. Phys. Letters **11**, No. 2, 62–64 (July 15, 1967).

Second breakdown—A comprehensive review, H. A. Schafft, Proc. IEEE **55**, No. 8, 1272–1288 (Aug. 1967).

Single- and double-quantum photodetachment of negative ions, E. J. Robinson and S. Geltman, Phys. Rev. **153**, No. 1, 4–8 (Jan. 1967).

Sporadic-*E* ionization, E. K. Smith, Annual Suppl. Encyclopedic Dictionary of Physics, Ed. J. Therolis, Suppl. I, 239–331 (Pergamon Press Inc., New York, N.Y., 1966).

Superconductive properties of ceramic mixed titanates, J. F. Schooley, H. P. R. Frederikse, W. R. Hosler, and E. R. Pfeiffer, Phys. Rev. **159**, No. 2, 301–305 (July 10, 1967).

Suppressed and accelerated spin-lattice relaxation, R. L. Peterson, Phys. Rev. **159**, No. 2, 227–233 (July 10, 1967).

Synchrotron radiation measurements near the magnetic equator, G. R. Ochs, Book, Radiation Trapped in the Earth's Magnetic Field, Ed. B. McCormac, pp. 703–713 (D. Riedel Publ. Co., Dordrecht, The Netherlands, 1966).

Temperature dependence of the nuclear quadrupole resonance frequency of ^{35}Cl in $KClO_3$ between 12° and 90° K, D. B. Utton, J. Chem. Phys. **47**, No. 2, 371–373 (July 15, 1967).

The energies of N^+ from the dissociative ionization of N_2 (Abstract), L. J. Kieffer and R. J. Van Brunt (Proc. 18th Annual Gaseous Electronics Conf., Minneapolis, Minn., Oct. 21, 1965), Bull. Am. Phys. Soc. **11**, No. 4, 499 (1966).

The radiative band pinch effect and temperature dependence of radiative recombination in GaAs, N. N. Winogradoff, K. Owen, and R. M. Curnutt, Int. J. Electronics **22**, No. 3, 229–233 (Mar. 29, 1967).

The use of multiple antennas in studies of absorption at conjugate points, H. J. A. Chivers and J. K. Hargreaves, Proc. Symp. High Latitude Particles and the Ionosphere, Alpbach, Austria, 1964, pp. 257–264 (Academic Press Inc., New York, N.Y., 1965).

Variational Calculations for quartet states of three-electron atomic systems, S. Geltman and E. Holein, Phys. Rev. **153**, No. 1, 81 (1967).

A comparison between solar X-ray emission and VLF sudden phase anomalies, C. J. Chilton, J. P. Conner, and F. K. Steele, Proc. IEEE **53**, No. 12, 2018–2026 (Dec. 1965).

Another method of synthesizing nonuniformly spaced antenna arrays, M. T. Ma, Trans. IEEE Ant. Prop. **AP-13**, No. 5, 833–834 (Sept. 1965).

Antennas, H. V. Cottony, Encyclopedia of Physics, Ed. R. M. Besancon, pp. 25–28 (Reinhold Publ. Co., New York, N.Y. 1966).

Some radio-physical considerations in studies of the fine scale structure of the atmosphere, B. R. Bean and B. D. Warner, Proc. Intern. Conf. Fine Scale Structure of the Atmosphere, Moscow, USSR, June 1965, pp. 215–224 (1965).

The application of the partial correlation analyses to the study of the occurrence probability of spread-*F*, T. Shimazaki (Proc. AGARD Conf. Spread *F* and Its Effects Upon Radiowave Propagation and Communication, Copenhagen, Denmark, Aug. 1964), AGARDograph **95**, pp. 167–188 (W. and J. Mackay, London, England, 1966).

The development of an International atomic time scale, J. A. Barnes, Proc. IEEE **55**, No. 6, 822–826 (June 1967).

The effect of spread *F* on the propagation of radiowaves near the equator, K. Davies and A. F. Barghausen (Proc. AGARD Conf. Spread *F* and Its Effects Upon Radiowave Propagation and Communication, Copenhagen, Denmark, Aug. 1964), AGARDograph **95**, pp. 437–466 (W. and J. Mackay, London, England, 1966).

**Publications for which a price is indicated are available by purchase from the Superintendent of Documents, U.S. Government Printing Office, Washington, D.C. 20402 (foreign postage, one-fourth additional). The NBS nonperiodical series are also available from the Clearinghouse for Federal Scientific and Technical Information, Springfield, Va. 22151. Reprints from outside journals and the NBS Journal of Research may often be obtained directly from the authors.*

U.S. GOVERNMENT PRINTING OFFICE : 1968 OL—289-930

UNITED STATES
GOVERNMENT PRINTING OFFICE
DIVISION OF PUBLIC DOCUMENTS
WASHINGTON, D.C. 20402

OFFICIAL BUSINESS

POSTAGE AND FEES PAID
U.S. GOVERNMENT PRINTING OFFICE

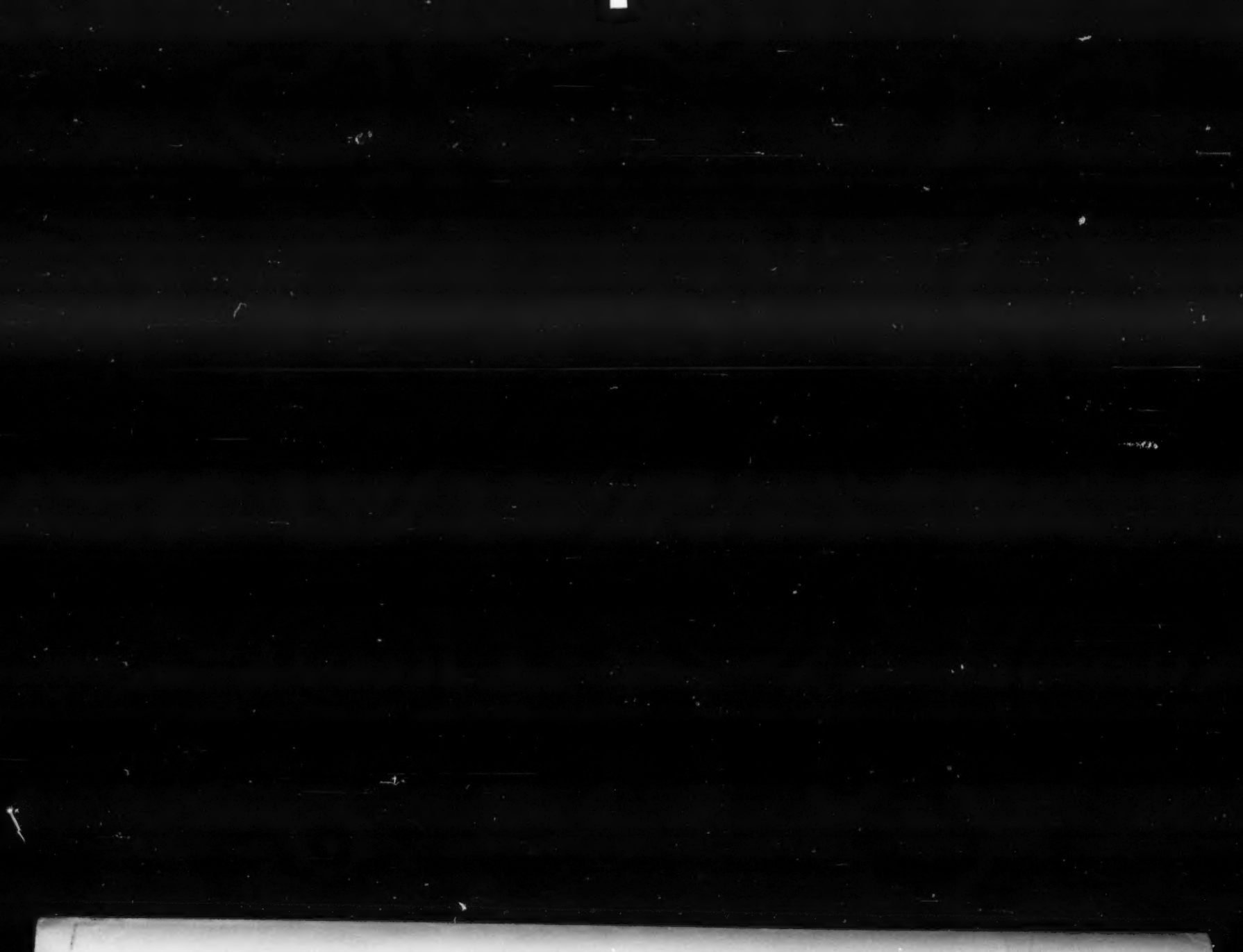
MIAMI UNIVERSITY LIBRARY

JOURNAL OF RESEARCH of the National Bureau of Standards Vol. 72B, No. 1 January–March 1968
B. Mathematical Sciences

Contents

	Page
Means and the minimization of errors. Michael Aissen.	1
On Taylor's theorem. O. Shisha.	
Principal submatrices III: Linear inequalities. R. C. Thompson.	7
The diophantine equation $P(x, y)=(xy+d)z$. Charles F. Osgood.	23
A note on the G-transformation. H. L. Gray and T. A. Atchison.	29
The distribution of the sample correlation coefficient with one variable fixed. David Hogben.	33
Solutions of the time-dependent Klein-Gordon and Dirac equations for a uniform electric field. Vernon W. Myers.	37
Analysis of a market split model. J. M. McLynn, A. J. Goldman, P. R. Meyers, and R. H. Watkins.	43
Citation searching and bibliographic coupling with remote on-line computer access. Franz L. Alt and Russell A. Kirsch.	61
Simple analytic expressions for the total Born approximation cross section for pair production in a coulomb field. L. C. Maximon.	79
Publications of the National Bureau of Standards.	89

Library of Congress Catalog Card Number: 62–4414

For sale by the Superintendent of Documents, U.S. Government Printing Office, Washington, D.C. 20402. Price 75¢ (single copy). Subscription price: $2.25 a year; 50¢ additional for foreign mailing.

UNITED STATES GOVERNMENT PRINTING OFFICE, WASHINGTON : 1968